Maidor Ali Controls

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Classical Mechanics deals with the macroscopic systems, i.e., the systems containing huge number of atoms or molecules and are directly observable or observable with the help of instruments like microscope. In the end of 19th century, with the discovery of electrons, X-rays, and radio-activity, the possibility arose of studying the individual atoms and molecules. It was then seen that classical theory was unable to explain the properties of atoms and molecules and their interactions with electromagnetic radiation. As a result of the efforts to modify the laws of classical physics, so that they can explain the behaviour of atoms and molecules, a new theoretical discipline, called the quantum theory, was developed by Schrodinger, Heisenberg, Dirac and others. We begin this chapter by discussing the difficulties encountered in explaining a few of the atomic phenomena by classical theory and the subsequent quantum mechanical explanation for them.

1.1. BLACK BODY RADIATION:

A perfectly black body is one which absorbs totally all the radiation of any wavelength which fall on it. Since, whatever the colour of incident radiation may be, it neither reflects nor transmits any radiation, it appears black. On the other hand, when such a body is heated to some temperature, it emits radiation of all possible wavelengths, called the black-body radiation. Lummer and Pringsheim (1899) made experiments to determine the distribution of energy among radiation of different wavelengths emitted by a black-body at various temperatures. Their results are depicted in Fig. 1. A close investigation reveals the following important facts:

- distributed in the radiation spectrum.
- (ii) At a given temperature, the intensity of radiation increases with increase in wavelength and becomes maximum at a

particular wavelength. With further increase in wavelength intensity decreases.

(iii) An increase in temperature causes a decrease in Am, the wavelength for which energy emitted is maximum.

In order to explain the observed spectra by applying the classical thermodynamics, it was shown by Wien that the amount of energy contained in the spectral region included within the wavelength λ and $\lambda + d\lambda$ emitted by a black-body is given by

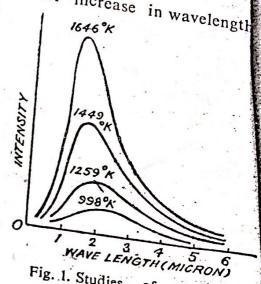


Fig. 1. Studies of black-body radiations by and Pringsheim. Lummer

$$E_{\lambda} d\lambda = \frac{A}{\lambda^5} e^{-C_{\lambda} T} d\lambda,$$

Where A and C are constants.

This formula works well only for short wavelengths. $\cdot \cdot (1)$ are considerable deviations from it at long wavelengths and high temperatures. Equation (1) gives finite energy even for $T=\infty$. Lord Rayleigh argued that it is, unlikely that E should be finite for infinite value of temperature.

Rayleigh and Jeans, by assuming that the radiation in blackbody have degrees of freedom and applying the law of equipartition of energy showed that $E_{\lambda} d\lambda = \frac{A}{\lambda^4} T d,$

$$E_{\lambda} d\lambda = \frac{A}{\lambda^4} T d^{-1},$$
ant. ...(2)

Where A is a constant. It is clear from this formula that the energy radiated in a given wavelength range $d\lambda$ increases rapidly as λ decreases and approaches infinity for very short wavelengths, which cannot be true. Thus the formula (2) holds good in the region of longer wavelengths but fails for the shorter wavelengths.

From the above discussion we see that the classical theory is unable to explain the black body radiation. In order to explain it. Planck put forward his quantum hypothesis, according to which -a black-body contains simple harmonic oscillators which are

capable of vibrating with all possible frequencies. The frequency of a radiation emitted by an oscillator is the same as the frequency of its vibration. An oscillator cannot emit energy in a continuous manner, it can emit energy in the multiples of the unit called quantum. If an oscillator is vibrating with a frequency v, it can only radiate in quanta of magnitude hv where h is a constant, called Planck's constant and its value is 6.625×10^{-27} erg-sec.

If N is the total number of Planck's oscillator and E is their total energy, then the average energy per oscillator is given by

$$\vec{\epsilon} = \frac{E}{N}$$
 ...(3)

Let N_0 , N_1 , N_2 , ..., N_n , ... etc. be the number of oscillators having energies 0, $\epsilon = h\nu$, 2ϵ , ..., $n\epsilon$, ... etc., respectively, then

$$N = N_o + N_1 + ... + N_n + ... = \sum_{n=0}^{\infty} N_n$$
 ...(4)

and
$$E = \epsilon (N_1 + 2N_2 + ... + nN_n + ...) = \sum_{n=0}^{\infty} n \epsilon N_n ...(5)$$

According to Maxwell's distribution formula, the probability for an oscillator to possess an energy E is given by

$$\exp(-E/kT)$$
.

Hence the average energy per oscillator can be written as

$$\frac{E}{\epsilon} = \frac{E}{N} = \frac{\sum_{n=0}^{\infty} n\epsilon e^{-n\epsilon/kT}}{\sum_{n=0}^{\infty} e^{-n\epsilon/kT}} \dots (6)$$

Putting $e^{-\epsilon/kT} = x$, we have

$$\sum_{n=0}^{\infty} e^{-n\epsilon/kT} = 1 + x + x^2 + \dots = \frac{1}{1-x} = \frac{1}{1-e^{-\epsilon/kT}}$$

and
$$\sum_{n=0}^{\infty} n\epsilon e^{-n\epsilon/kT} = \epsilon \left(x + 2x^2 + 3x^3 + \dots \right)$$

$$= x\epsilon \frac{d}{dx} (1 + x + x^2 + \dots)$$

$$= x\epsilon \frac{d}{dx} \left(\frac{1}{1 - x} \right) = \frac{x\epsilon}{(1 - x)^2}$$

$$= \frac{\epsilon e^{-\epsilon/kT}}{(1 - e^{-\epsilon/kT})^2}.$$

$$\therefore \quad \overline{\epsilon} = \frac{\epsilon e^{-\epsilon/kT}}{1 - e^{-\epsilon/kT}} = \frac{\epsilon}{e^{\epsilon/kT} - 1} = \frac{h\nu}{e^{h\nu/kT} - 1}. \quad ...(7)$$

Now, the number of oscillators per unit volume in the frequency range v to v+dv is given by

$$N = \frac{8\pi v^2 dv}{c^3} \qquad \dots (8)$$

Multiplying it by the average energy per oscillator, given by equation (7), we get the total energy per unit volume belonging to range dv or the energy density belonging to range dv as

$$E_{v} dv = \frac{8 \cdot hv^{3}}{c^{3}} \cdot \frac{1}{e^{hv/\mu T} - 1} dv. \qquad ...(9)$$

This is known as Planck's radiation law.

This law can be represented in terms of wavelength as

$$v = \frac{c}{\lambda} \text{ and } |dv| = \left| \frac{-c}{\lambda^2} d\lambda \right|,$$

$$\therefore E_{\lambda} d\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{ch/\lambda kT} - 1} d\lambda. \qquad ...(10)$$

Planck's radiation law explains all the observed facts of the black-body spectrum for the entire wavelength range.

For small temperatures and short wavelengths, λT is small and hence, echint >> 1. Therefore, 1 can be neglected in the denominator of equation (10). Hence,

$$E_{\lambda} d\lambda = \frac{8\pi hc}{\lambda^5} e^{-hc/\lambda kT} d\lambda. \qquad ...(11)$$

This is Wien's law, with $A=8\pi ch$ and $C=\frac{-hc}{k}$.

For high temperatures and large wavelengths, λT is large. Therefore,

$$e^{hc/lk\lambda T} \approx 1 + \frac{hc}{\lambda kT}$$

Using it into (10), we get

$$E_{\lambda} d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda. \qquad ...(12)$$

This is the Rayleigh-Jeans law with $A=8\pi k$.

Above description illustrates that Planck's law is perfect one and all other laws follow as special cases of this law, which account only for limited portion of the black-body spectrum.

PHOTO-ELECTRIC EFFECT:

Liberation of electrons from matter under the influence of sufficiently high frequency electromagnetic radiations is known

as photoelectric effect. Experimental studies of photoelectric effect show that:

- (i) For light of any given frequency, the photoelectric current is directly proportional to the intensity of light, provided the frequency is above the threshold frequency.
- (ii) For a given photosensitive material, there is a certain minimum frequency, called the threshold frequency, below which the emission of photoelectrons stops completely, no matter how great is the intensity of light.
- (iii) The photoelectric emission is an instantaneous process. As soon as the frequency of light exceeds the threshold frequency, the emission starts immediately without any apparent lag.
- (iv) The maximum kinetic energy of the photo-electrons is found to increase with the increase in the frequency of the incident light provided the frequency exceeds the threshold limit. maximum kinetic energy is, however, found to be independent of the intensity of light.

The above laws of photoelectric emission could not be accounted for by the classical wave theory of light. According to classical considerations, more intense radiation, having a stronger electric field, would produce more energetic electrons. to this, the energy of the photoelectrons is independent of the intensity of the incident light. Also, the existence of a threshold is difficult to explain. On the basis of the wave theory of light, the energy of wave is distributed equally over the entire wavefront, whereas, the electron has a very small target area. Calculations show that in case of sodium, the time required for a photoelectron to absorb the energy of emission would be more than 100 days, whereas, experimentally the effect is almost instantaneous.

In 1905, Einstein proposed a theory based upon Planck's idea of quanta of energy which gave a satisfactory explanation of the various experimental facts. According to him, monochromatic light of frequency ν consists of photons of energy $h\nu$, where h is Planck's constant. When a photon with a sufficient energy content strikes an electron of a photosensitive material, a part of its energy known as the work function W_0 of the surface, is used up in liberating the electron from the surface, whereas, the remaining is spent in imparting kinetic energy to it. If m is the mass and v

ADVANCED QUANTUM THEORY AND FIELDS the maximum velocity of the emitted electron, then

$$hv = W_0 + \frac{1}{2}mv^2$$
.

This is known as Einstein's photo-electric equation. ...(13)

The maximum kinetic energy of the emitted electrons is given from equation (13) as

 $\frac{1}{2}mv^2 = (hv - W_0).$

It follows from equation (14) that the maximum velocity of the emitted electron depends upon the frequency of the incident radiation. An increase in the frequency of the incident light increases the amount of energy carried by each individual light quantum so that, during each collision with a free electron in the metal, these quanta impart larger amount of kinetic energy. An increase in the intensity of light cannot cause any change in the kinetic energy (or the maximum velocity) of the emitted electrons. More intense light simply means more number of light quanta having the same energy falling on the surface per sec. Since one light quantum can emit only one electron, the number of electrons emitted will correspondingly increase.

Further, if vo is the lowest or threshold frequency which just causes the emission of electrons, then we have

$$hv_0 = W_0$$

therefore equation (14) reduces to

$$\frac{1}{2}mv^2 = h (v - v_0).$$
(15) that no photon 1...(15)

It is evident from eqn. (15) that no photoelectric effect is possible if $v < v_0$, i.e, the frequency of the incident radiation is less than the threshold frequency. Thus the Einstein's treatment of photoelectric effect, based on Planck's idea of quanta of energy, satisfactorily explains all the experimental facts about photoelectric emission.

1.3. SPECIFIC HEAT OF SOLIDS:

According to the classical theory of matter, the mean kinetic energy per degree of freedom at temperature T is $\frac{1}{2}kT$. A solid may be supposed to consist of individual atoms which are bound to their neighbours, but they can vibrate freely when heated. Now, each atomic oscillator will have three degrees of freedom of oscil-Thus the kinetic energy of oscillation of all the atoms in one gram atom of a solid will be

N. $\frac{3}{2}kT = \frac{3}{2}RT$:

N is Avogadro's number and R is the molar gas constant.

The mean potential energy for each of the three components of vibration is also equal to $\frac{1}{2}kT$; since the kinetic energy is equal to the potential energy for a simple harmonic oscillator. Therefore, the potential energy of each atomic oscillator is $\frac{3}{2}kT$. Hence, the potential energy for one gram atom is given by

$$N._{2}^{3} kT = \frac{3}{2}RT.$$

Therefore, the total energy of one gram atom of a solid is given by

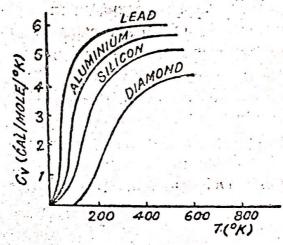
$$E=\frac{3}{2}RT+\frac{3}{2}RT=3RT.$$
 ...(16)

Hence the specific heat at constant volume is

$$C_{\nu} = \left(\frac{\partial E}{\partial T}\right)_{\nu} = 3R. \tag{17}$$

Thus the specific heat for all the solids at all the temperatures comes out to be 3R, but for a number of substances it was found to be much smaller than 3R. Moreover, it was found to vary with temperature, tending to zero at absolute zero. Fig. 2 represents the variation of specific heat with temperature for some solids. Thus the

heat of solids with temperature.



classical theory is unable to explain the behaviour of the specific

Einstein tried to explain this by applying the planck's quantization hypothesis. He pointed out that the average energy of an oscillator, vibrating with frequency v, is not kT per degree of vibration, rather it is given by an expression identical to that for Planck's black body oscillators, viz, eqn (7). Under this assumption, the total energy of one gram atom of the solid will be given by

$$E=3N. \frac{h\nu}{e^{h\nu/kT}-1}$$

$$\therefore C_{\nu} = \left(\frac{\partial E}{\partial T}\right)_{\nu} = 3R \left(\frac{h\nu}{kT}\right) \frac{e^{h\nu/kT}}{(e^{h\nu/rT}-1)^2} \qquad (18)$$
At high temperatures, $\frac{h\nu}{kT} \to 0$, and $(e^{h\nu/kT}-1)^2 \approx {h\nu \choose kT}^2$.

Therefore, $C_{\nu} \approx 3R$, in agreement with the kinetic theory.

When T-0, $\frac{hv}{kT} \to \infty$ and hence we can neglect unity in comparison to $e^{hv/kT}$ in the denominator. Therefore, we get

$$C_{\nu} \cong 3R \frac{e^{h\nu/kT}}{e^{2h\nu/kT}} \left(\frac{h\nu}{kT}\right)^{2} = 3R \frac{1}{e^{h\nu/kT}} \left(\frac{h\nu}{kT}\right)^{2}$$

$$= 3R \left[\frac{(h\nu/kT)^{2}}{1 + \frac{h\nu}{kT} + \frac{1}{2!} \left(\frac{h\nu}{kT}\right)^{2} + \dots}\right] \qquad \dots (19)$$

From it we see atonce that $C_{\nu} \to 0$ as $T \to 0$. This is also in general agreement with the experimental results.

Though the Einstein's theory predicts almost correctly the variation of specific heat with, temperature, it was observed that in the case of certain elements like copper, aluminium etc. the atomic heat at low temperatures decrease more rapidly than that predicted by equation (18). This disagreement, is due to the assumption of monochromatic vibration, i.e., due to the assumption that all the atoms of the solid vibrate with one and the same frequency. In reality, atoms exert forces on each other and hence every oscillator is under the field of thousands of other vibrating atoms. Debye modified the Einstein's theory which gives excellent agreement with the observations over the entire temperature range.

Dbye assumed that a solid vibrates elastically with a continuous spectrum of frequencies. When a continuous solid is thrown into elastic vibrations, two kind of waves are excited in it

(a) transverse vibrations, which travel with the velocity $v_i = \sqrt{\left(\frac{\eta}{\rho}\right)}$ and (b) longitudinal vibrations, which travel with the velocity $v_i = \sqrt{\{(K + \frac{4}{3}\eta)/\rho\}}$,

where η is the coefficient of rigidity, K the bulk modulus and ρ the density of the solid.

The number of modes of longitudinal vibrations per unit volume with frequencies between v and $v+dv=\frac{4\pi v^2}{v_i^2}\frac{dv}{v_i^2}$

The number of modes of transverse vibrations per unit volume with frequencies between ν and $\nu + d\nu = 2 \times \frac{4\pi \nu^2 d\nu}{v_i^3}$, the multiplication factor of 2 appears because the transverse vibrations have

two independent direction of vibrations, i.e., they are equivalent to two waves polarized at right angle to each other.

Therefore, the total number of independent modes of vibrations per unit volume with frequency between v and v+dv is given by

$$4\pi v^2 \left(\frac{1}{v_1^3} + \frac{2}{v_1^3}\right) dv.$$

If V be the volume of one gram atom of the solid, the number of modes of vibrations for this amount within frequencies v to v+dv will be

$$4\pi v^2 V \left(\frac{1}{v_t^3} + \frac{2}{v_t^3}\right) dv.$$

Therefore, the total number of independent modes of vibrations in the entire frequency spectrum is given by

or
$$\int_{0}^{v_{m}} 4\pi V \left(\frac{1}{v_{l}^{3}} + \frac{2}{v_{l}^{3}}\right) v^{2} dv = 3N$$

$$4 \cdot V \left(\frac{1}{v_{l}^{3}} + \frac{2}{v_{l}^{3}}\right) \frac{v_{m}^{3}}{3} = 3N$$
or
$$v_{m}^{3} = \frac{9N}{4\pi V \left(\frac{1}{v_{l}^{3}} + \frac{2}{v_{l}^{3}}\right)} \cdot \dots (20)$$

The elastic spectrum is thus cut at an upper limit v_m which has a definite value for each substance.

The total energy of the solid is, therefore, given by

$$E = 4\pi V \left(\frac{1}{v_i^3} + \frac{2}{v_i^3} \right) \int_0^{v_m} \frac{hv}{e^{hv/kT} - 1} v^2 dv$$

$$= \frac{9N}{v_m^3} \int_0^{v_m} \frac{hv^3 dv}{e^{hv/kT} - 1} \text{ [using eqn. (20)]}.$$

Let $\frac{hv}{kT} = x$, then $v = \frac{kT}{h}x$ and $dv = \frac{kT}{h}dx$. Let us also define

a characteristic temperature $T_c = \frac{h v_m}{k}$, so that $v_m = \frac{k T_c}{h}$. Then,

$$E = 9RT \left(\frac{T}{T_c}\right)^3 \int_0^{T_c/T} \frac{x^3}{e^x - 1} dx.$$

$$\therefore C_V = \left(\frac{\partial E}{\partial T}\right)_V = 9R \left[4 \left(\frac{T}{T_c}\right)^3 \int_0^{T_c/T} \frac{x^3 dx}{e^x - 1} + \frac{(T_c/T)^3}{e^{T_c/T} - 1} \cdot \left(\frac{-T_c}{T^3}\right) \right]$$

$$= 9R \left[4 \left(\frac{T}{T_c}\right)^3 \int_0^{T_c/T} \frac{x^3 dx}{e^x - 1} - \frac{T_c}{T} \cdot \frac{1}{e^{T_c/T - 1}} \right] \dots (21)$$

For high values of T, x and T_c/T are very small and hence $e^x \approx 1 + x$ and $e^{T_c/T} \approx 1 + \frac{T_c}{T}$. Therefore,

$$C_{V} \cong 9R \left[4 \left(\frac{T}{T_{c}} \right)^{3} \int_{0}^{T_{c}/T} x^{2} dx - 1 \right] = 9R \left[\frac{4}{3} - 1 \right] = 3R.$$

At very low temperature, $x\to\infty$ and $\frac{T_c}{T}\to\infty$. Hence, the last term in (21) can be neglected and the first term can be written as

$$C_{V} \approx 9R.4 \left(\frac{T}{T_{c}}\right)^{3} \int_{0}^{\infty} \frac{x^{3} dx}{e^{x} - 1} = 36R \left(\frac{T}{T_{c}}\right)^{3} \left(\frac{\pi^{4}}{15}\right) \approx 234 \left(\frac{T}{T_{c}}\right)^{3}$$

Thus at low temperature, the specific heat varies as 73.

This is known as Debye's T3 law.

For intermediate temperatures, integral in eqn. (21) is evaluated numerically. It has been found that Debye's formula explains quite successfully the observed variation of specific heat of solids.

1.4. HYDROGEN SPECTRUM:

In 1911, Rutheford from his α particle scattering experiment concluded that the atom is consisted of a central positively charged massive nucleus around which the electrons rotate in circular orbits. The centripetal force for rotation being provided by the electrostatic force of attraction between the nucleus and the electron. Since the electrons are subjected to centripetal acceleration while rotating in orbits around the nucleus, according to classical electromagnetic theory, they will loose energy by radiating at the rate $P = \frac{e^2 a^2}{6\pi\epsilon_0 c^3}$ watts, where a is the acceleration. Consequently, the electrons should spiral in towards the nucleus and ultimately collapse into it, which is not the case in reality.

In order to explain this, *Bohr*, applied the quantization rule to the Rutherford's model of atom and successfully explained the observed spectum of hydrogen atom. According to Bohr, an electron in an atom can rotate only in a number of allowed circular orbits around the nucleus and these circular orbits are such that the orbital angular momentum of the electron in the orbit is an integral multiple of $h/2\pi$; where h is Flanck's constant.

Thus, the Bohr's quantization condition is

$$mrv = n \frac{h}{2\pi}$$
 or $2\pi mrv = nh$(22)

Here,
$$n=1, 2, 3, ..., \infty$$
.

Also, for an electron rotating in an orbit of-radius r, the centripetal force acting on it will be mv^2/r . If Ze is the charge of nucleus, the electrostatic force on the electron will be Ze^2/r^2 . Hence, we have

$$\frac{Ze^2}{r^2} = \frac{mv^2}{r} \qquad \dots (23)$$

From equations (22) and (23), we have

$$v = \frac{2\pi Ze^2}{nh} \cdot \dots (24)$$

and

$$r = \frac{n^2 h^2}{4\pi^2 Z e^2 m} \qquad ...(25)$$

The total energy E_n is equal to the sum of the kinetic energy and the potential energy,

$$E_n = \frac{1}{2}mv^2 - \frac{Ze^2}{r} \qquad ...(26)$$

Using eqn (23) into (26), we obtain

$$E_n = -\frac{1}{2} \frac{Ze^2}{r} = -\frac{1}{2} mv^2 \qquad ...(27)$$

Putting the value of v from eqn. (24) into eqn. (27),

$$E_n = -\frac{2\pi^2 Z^2 e^4 m}{n^2 h^2} \cdot \dots (28)$$

When correction is made for the motion of the proton around the centre of mass of the hydrogen atom, the energy for the system becomes,

$$E_n = -\frac{2\pi^2 Z^2 e^4 \mu}{n^2 h^2}, \qquad ...(29)$$

where μ is the reduced mass of the proton-electron system Bohr postulated that the radiation are emitted only when an electron jumps from one of the allowed orbit to another lower orbit If the electron jumps from the orbit of energy E_{n1} to a lower orbit of energy E_{n2} , the frequency of emitted radiation is given by

$$v = \frac{E_{n_1} - E_{n_2}}{h} = \frac{2\pi^2 m e^4}{h^3} Z^2 \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right).$$

Wave number $\overline{\nu}$ of this radiation is

$$\overline{v} = \frac{1}{\lambda} = \frac{v}{c} = \frac{2\pi^2 m e^4}{ch^3} Z^2 \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right)
= RZ^2 \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right), \quad ...(30)$$

where $R = \frac{2\pi^2 me^4}{ch^3} \approx 109$, 677 cm⁻¹ is the Rydberg's constant.

There is striking agreement between the frequencies of the various observed spectral lines and those given by eqn. (30). For $n_1=2$ and $n_2=3$, 4, 5,...etc, we obtain the $H_{\alpha},H_{\beta},...$ etc. spectral lines of the Balmer's series. Similarly for $n_1=1$, 3, 4, 5 and $n_2=2$, 3, 4,...etc.; 4, 5, 6, ...etc.; 5, 6, 7,...etc.; 6, 7, 8,...etc; respectively, we obtain the spectral lines of the Lyman, Paschen, Brackett and Pfund's series; respectively.

1.5 COMPTON SCATTERING:

Compton (1923) found that when a beam of monochromatic X-rays is scattered from some light element, the scattered beam at various angles have a frequency lower than that of incident rays or a wavelength greater than that of the incident beam

According to classical mechanics, the electric field of the incident electromagnetic wave train exerts a force on the atomic electrons in the scattering material and set them into forced vibrations of the same frequency as that of the incident waves. The oscillating electrons will then emit rays of frequency equal to their own; like an oscillating electric dipole. The scattered rays should thus be identical in wavelength with the incident waves. Hence the classical mechanics is inadequate in explaining the Compton scattering.

Theoretical interpretation of the decreases in frequency or in crease in wavelength was given by Compton himself on the basis of Einstein's photon hypothesis. He considered the scattering process as an elastic collision between a photon and an electron of scattering material. As shown in Fig. 3, let the X-rays consist of photons or quanta of energy hy where v is the frequency. The momentum of the photon of energy h_v will be h_v/c . Let m_0 be the rest mass of the electron and thus m_0c^2 its rest mass energy. initial momentum is zero During the collision, a part of the energy of the photon is imparted to the electron which acquires a velocity v along a direction making an angle θ with the direction of motion of incident photon After having lost some energy, the photon is left with smaller energy hv' (and hence a lower frequency v') and gets scattered along a direction making an angle & with its orginal direction. The electron moving with velocity v will have a mass,

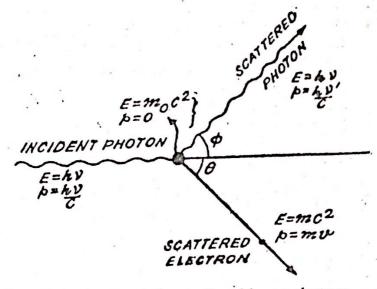


Fig. 3. X-ray photon being scattered by an electron.

$$m = \frac{m_0}{\left(1 - \frac{v^2}{c^2}\right)^{1/2}}$$

The electron thus has energy equal to mc2 and momentum mv,

From the principle of conservation of energy, we have

$$h_{\nu} + m_{0}c^{2} = h_{\nu}' + mc^{2}$$

 $mc^{2} = m_{0}c^{2} + h(\nu - \nu')$

or

Squaring both sides

$$m^{2}c^{4} = m_{0}^{2}c^{4} + h^{2}(v - v)^{2} + 2m_{0}^{2}c^{2}h(v - v') \qquad \qquad \therefore (31)$$

Applying the principle of conservation of momentum in the original direction of the incident photon, we have

$$\frac{h_{V}}{c} + 0 = \frac{h_{V}'}{c} \cos \phi + mv \cos \theta \qquad ...(32)$$

Applying this law along perpendicular direction, we get

$$0 = \frac{hv'}{c} \sin \phi - mv \sin \theta \qquad ...(33)$$

From (32) and (33), we have,

 $mvc\cos\theta = hv - hv'\cos\phi$

and

 $mvc \sin \theta = hv' \sin \phi$

Squaring and adding these equations, we obtain $m^2v^2c^2(\cos^2\theta+\sin^2\theta)=h^2v^2+h^2v'^2\cos^2\phi-2h^2vv'\cos\phi+h^2v'^2\sin^2\phi$

or
$$m^2v^2c^2=h^2 (v^2+v'^2-2vv'\cos\phi)$$
 ... (34)
Subtracting (34) from (31), we get $m^2c^2 (c^2-v^2)=m_0^2c^4-2vv'h^2 (1-\cos\phi)+2m_0c^2 h(v-v')$

Putting
$$m = m_0 / \sqrt{\left(1 - \frac{v^2}{c^2}\right)}$$
 into this equation, we get
$$m_0^2 c^4 = m_0^2 c^4 - 2vv' \ h^2 \left(1 - \cos \phi\right) + 2m_0 c^2 h \ (v - v')$$
or
$$2vv' \ h^2 \left(1 - \cos \phi\right) = 2m_0 c^2 h \ (v - v')$$
or
$$\frac{v - v'}{vv'} = \frac{h}{m_0 c^2} \left(1 - \cos \phi\right)$$

$$\frac{c}{v'} - \frac{c}{v} = \frac{h}{m_0 c} \left(1 - \cos \phi\right)$$
or
$$\Delta \lambda = \lambda' - \lambda = \frac{h}{m_0 c} \left(1 - \cos \phi\right). \qquad ...(35)$$

Thus the wavelength λ' of the scattered photon is greater than that of the incident photon by an amount $\Delta\lambda$, given by eqn. (35). Experimental values of $\Delta\lambda$ are found to be in good agreement with that given by eqn. (35). The important theoretical fact is that it was obtained by considering the light quantum or photon as a particle.

1.6. WAVE PARTICLE DUALITY:

It has been seen that the phenomena like photoelectric effect and the Compton effect could be explained if electromagnetic 4 radiation was supposed to consist of packets of energy called quanta or photons which behaved like particles and moved through space with the velocity of light. It is also well known that light exhibits the phenomena of interference, diffraction and polarization, which can only be explained by wave nature of light. Radiation was thus regarded as exhibiting a dual wave-particle behaviour and the physicist made use of either the wave or the particle nature of light to explain an experimental phenomenon as it suited them. This fact led Louis de Broglie to make in 1924 a daring suggestion that if light which is known to consist of waves can, under certain circumstances, assume the aspect of a particle, then the particle of matter should also behave like waves. He based his reasoning on the assumption that nature loves symmetry and that the two physical entities, matter and wave must be symmetrical. de Broglie's suggestion about the wavenature of particles was verified experimentally by Davission and Germer in 1927 and G.P. Thomson in 1928, and thus the truth of his assertion was established.

Now, if the material particles behave like wave, then what is the wavelength of the associated wave? As already seen, the energy of a photon of radiation of frequency v is given by E=hv, where h is Planck's constant. If the photon is considered to be a particle of mass m, its energy will be equal to mc^2 , where c is the velocity of light. Thus.

$$hv = mc^2$$
 ...(36)

From eqn. (36) we have

$$mc = \frac{hv}{c} = \frac{h}{\lambda} \left\{ : \frac{c}{v} = \lambda \text{ is the wavelength of the radiation} \right\}$$

or
$$\lambda = \frac{h}{mc} = \frac{h}{p}$$
, ...(37)

where p=mc is the momentum of the photon.

de Broglie assumed that eqn. (37) should equally be applicable to both the photons of radiation and other material particles. If a particle of mass m moves with a velocity v, then the wavelength of the wave associated with it should be given by

$$\lambda = \frac{h}{p} = \frac{h}{mv}.$$
 (38)

Eqn. (38) is known as de Broglie wave equation and he derived it by picturing a material particle as a standing wave system in the vicinity of the particle. Let the standing wave at any instant t_0 at the point (x_0, y_0, z_0) be represented by the function

$$\psi = \psi_0 \sin 2\pi v t_0, \qquad \dots (39)$$

where v_0 is the frequency of the wave and ψ_0 its amplitude.

If the particle is now given a velocity v along the positive x-direction, then the variation of ψ will be given by replacing t_0 by $\frac{t-vx/c^2}{\sqrt{(1-v^2/c^2)}}$ in equation (39).

$$\therefore \ \psi = \psi_0 \sin \frac{2\pi v_0 (t - vx/c^2)}{\sqrt{(1 - v^2/c^2)}} \qquad ...(40)$$

Comparing equation (40) with the standard equation of wavemotion,

$$y = A \sin \frac{2\pi}{\lambda} (ut - x),$$

3

where A is the amplitude, λ the wavelength and u the velocity of the wave along the positive x-axis, we see that

$$u = \frac{c^2}{v}$$
 and $\frac{1}{\lambda} = \frac{v_0}{\sqrt{(1 - v^2/c^2)}} \cdot \frac{v}{c^2}$...(41)

From Einstein's mass energy relationship, we have $h_{\nu_0} = m_0 c^2$ or $\nu_0 = mc^2/h$

$$\frac{1}{\lambda} = \frac{m_0 c^2/h}{\sqrt{(1 - v^2/c^2)}} \cdot \frac{v}{c^2} = \frac{m_0}{\sqrt{(1 - v^2/c^2)}} \cdot \frac{v}{h} = \frac{mv}{h}$$

$$\left\{ \because m = \frac{m_0}{\sqrt{(1 - v^2/c^2)}} \right\}$$
or
$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

which is exactly the same as given by eqn. (38).

de Broglie's wave equation provides a physical basis to Bohar's empirical statement of discrete, non-radiating electronic energy states in an atom. According to Bohr.

$$mvr = n\frac{h}{2\pi}$$
or
$$2\pi r = n\frac{h}{mv} = n\lambda$$

Thus permitted orbits are only those whose length, $2\pi r$, is an integral multiple of the wavelength associated with the electron.

The Davisson and Germer Experiment. The particle waves predicted by de Broglie were first experimentally detected in 1927 by two American Physicists, Davisson and Germer. Their apparatus is shown schematically in Fig. 4. It consists of an electron gun

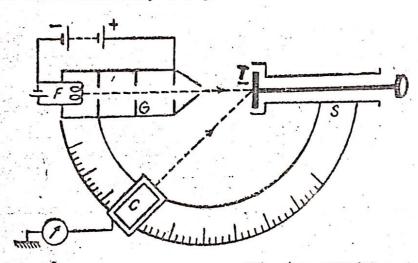


Fig. 4. Davission-Germer electron diffraction apparatus. Which comprises of a tungsten filament F heated by a low tension battery. The electrons emitted by the filament are accelerated in an electric field of known potential difference from a high tension battery. The electrons are collimated to a fine beain by allowing them to pass through suitable slits. This entire arrangement to produce a fine beam of electrons accelerated to a desired velocity is known as electron gun.

7:3

The collimated beam of electrons is made to strike a Nickel target T which is capable of rotation about an axis parallel to the axis of the incident beam. The electrons are scattered in all directions by the atoms of the crystal. The intensity of the electron beam scattered in a given direction is measured by allowing it to enter in a Faraday cylinder called the collector C, which can be moved along a graduated circular scale S, so that it is able to receive the reflected electrons at all angles between 20° and 90°. The collector is connected to a galvanometer whose deflection is proportional to the intensity of the beam entering the collector. The whole apparatus is enclosed in an evacuated chamber.

If the electrons of charge e e.s.u. is accelerated through a potential of V volts and attains a velocity v, then

$$\frac{1}{2}mv^2 = \frac{eV}{330}$$
; m is the mass of the electron.

$$m^2 v^2 = \frac{meV}{150} \text{ and } mv = \sqrt{\left(\frac{meV}{150}\right)}$$

From de Broglie's relation, we get

$$\lambda = \frac{h}{mv} = h \cdot \sqrt{\left(\frac{150}{meV}\right)}$$

Putting $h=6.55\times10^{-27}$ erg-sec., $m=9\times10^{-28}$ gm. and $e=4.77\times10^{-10}$ e.s.u. in this expression, we obtain

$$\lambda = \sqrt{\left(\frac{150}{V}\right)} \text{ Å.} \qquad \dots (42)$$

Thus, knowing the accelearating potential, we can calculate the wavelength of the electron-waves.

In one particular determination, an electron beam accelerated by a potential of 54 volts was directed upon a Nickel target and a sharp maxima in the electron distribution occured at an angle of 50° with the original beam. The incident and the scattered beam in this case make an angle of 65° with the family of Bragg's planes (see Fig. 5). The spacing of planes in this family, which can be determined by X-ray diffraction, is 0.91 Å. Applying Bragg's equation $2d \sin \theta = n\lambda$, for maximum in a diffraction pattern and taking n=1, we have

$$2 \times 0.91 \times \sin 65^{\circ} = 1.\lambda$$

 $\lambda = 1.65 \text{ Å}.$

Now applying de Broglie's formula, we have

$$\lambda = \sqrt{\left(\frac{150}{V}\right)} = \sqrt{\left(\frac{150}{54}\right)} = 1.66 \text{ Å} \quad \{\because V = 54 \text{ volts}\}.$$

There is an excellent agreement between the two results. Thus Davisson-Germer experiment provides a direct verification of de Broglie's hypothesis of the wave of moving particles.

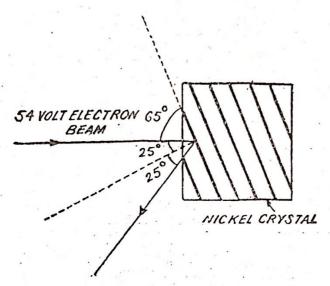


Fig. 5. Family of Bragg's planes

Experiment of G. P. Thomson:—Another experimental evidence for the existence of de Broglie's waves was given by G.P. Thomson. A beam of cathode rays is produced in a discharge tube and passed through suitable slits to obtain a fine pencil of electrons. The electrons are then accelerated under potentials varying from 10,000 to 50,000 volts and made to bombard against a thin film of metal like gold, silver, aluminium etc. After passing through the film, the cathode rays are received upon a photographic film or a fluorescent screen. The film or the screen shows a pattern consisting of a series of well defined concentric rings about a central spot, very much like that produced by X-rays in the powdered crystal method.

Let AB be the incident beam passing through the film at B. Let BE be the beam which has suffered a Bragg reflection and falls at the point E on the screen at a distance 'r' from the central spot C; as shown in Fig. 6. Let the distance BC from the film to the screen be D. The angle $CBE=2\theta$, where θ is given by Bragg's relation, $2d \sin \theta = n\lambda$. Taking θ very small, we can write it as $2d.\theta \approx n\lambda$. From Fig. 6 we have

r=D tan $2\theta \approx D.2\theta$; since θ and hence 2θ is very small.

or
$$r=D.\frac{2n\lambda}{2d} = \frac{Dn\lambda}{d}$$
 $\left\{ : 2d\theta = n\lambda \text{ or } \theta = \frac{n\lambda}{2d} \right\}.$

Equation (42) for λ with very high speed electrons can be written by applying the relativistic correction as:

$$\lambda = \sqrt{\left(\frac{150}{V}\right)} \cdot \left(1 + \frac{\alpha}{2}\right)^{-1/2}$$
, where $\alpha = \frac{eV}{300 \ m_0 c^2}$.

Substituting this value of λ we get

$$r = \frac{nD}{d} / \left[\frac{150}{V}\right] \cdot \left(1 + \frac{\alpha}{2}\right)^{-1/2} \tag{43}$$

Fig. 6. G. P. Thomson's experiment for electron diffraction.

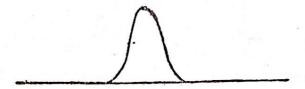
Putting the values of r, the radius of the diffraction ring; D, the distance of the screen from the film and V, the accelerating potential, we can calculate the grating space 'd'. The values of the grating space found from (43) in this way for various metals was in good agreement with those found by means of X-ray diffraction. Thus, the de Broglie's law was verified.

1.7. HEISENBERG'S UNCERTAINTY PRINCIPLE:

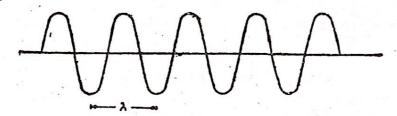
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In the preceding section we have seen that a moving particle with a well defined momentum p, behaves like a wave of wavelength $\lambda = h/p$, and that the state of the particle at any time can be specified by a wave function $\psi(x, y, z, t)$. According to Max Born, the absolute square of the wave function at a point gives the probability that the particle will be found, if we look for it with a detector, in the neighbourhood of the point. Thus, the particle will most likely be found in those regions of space in which the amplitude of the wave function is large. If the wave function of the particle is such that its amplitude is zero except in a very small region of space, we can say that the particle is in this region, i.e., its position is accurately known. On the other hand, if the wave function has non-zero amplitude over a very large region, we cannot assign a precise position to the particle.

Similar considerations apply to the momentum of the particle. From de Broglie's equation we see that the momentum cannot be well defined unless the wavelength is well defined. For the wavelength to be well defined, the wave function should be regular and periodic, As an example, a long sine wave has a well defined wavelength and hence a well defined momentum. But the position of the particle for a long sine wave cannot be accurately known. Contrary to this, if we have a wave function for which the position of the particle is well defined, i.e., the wavefunction has very large amplitude over a very small region of space and zero elsewhere, then the wavelength and hence the momentum of the particle cannot be defined precisely. This is illustrated in Fig. (7).



(a) Position very well defined, wavelength very poorly defined.



(b) Position poorly defined, wavelength well defined.

Fig. 7.

Thus, we are confronted with a problem of determining both the position as well as the momentum of a particle represented by a de Broglie wave. Heisenberg was the first to realise these consequences of the wave-particle duality. He stated that whereas there are no limits to the accuracy to which either the momentum or the position can be defined, there is a fundamental limit to the accuracy to which the position and the momentum can be defined simultaneously. He expressed it by the following equation, known as Heisenberg's Uncertainty relation

$$\triangle x. \triangle p_x \approx h$$
 ...(44

i.e., the product of the uncertainties in determining the position and momentum of a particle is approximately equal to Planck's constant. Although to it smaller the value of $\triangle x$, i.e., more exactly we determine the position, larger will be the value of

 Δp_x , i.e., less exactly we can determine the momentum. The converse is equally true.* Thus the accuracies to which the position and the momentum of a particle can be measured at a time are complementary to each other. This is, sometimes, also called the Complementarity Principle.

Though Heisenberg stated the uncertainty principle for position and momentum only, the relation is universal and holds good for all the canonically conjugate physical quantities like energy and time, angular momentum and angle etc. Thus, if ΔE is the uncertainty in determining the energy of the particle and Δt is that in determining the time to which this determination refers, then we must have

$$\triangle E. \triangle t \approx h$$
 ...(45)

Similarly,

 $\triangle J. \triangle \theta \approx h$...(46)

where $\triangle J$ and $\triangle \theta$ are the uncertainties in determining the angular momentum and the angle; respectively.

1.8. SUPERPOSITION PRINCIPLE AND CONSTRUCTION OF WAVE PACKET:

So far we have seen that a wave property is associated with a moving material particle and that the particle wave can be represented by an algebraic function of the space and time coordinates, called the wavefunction of the particle. Also, the wave like phenomena should be localized in the neighbourhood of the particle, so that the position of the particle can be defined. However, due to uncertainty principle, we cann't define the position of the particle very well. Hence, we can only represent the particle by a wave packet (see fig. 8) which can define the position of the particle to an accuracy of $\Delta x \Delta y \Delta z$ and hence the momentum to an accuracy of $\Delta p_x \Delta p_y \Delta p_z$, where Δx 's and Δp_x 's are related by the relations of the form (44).

*In order to restore these aspects of friendship, Schroedinger suggested that a particle whose position is defined to an accuracy of $\triangle x \triangle y \triangle z$ (in consistency with the uncertainty principle) can be represented by a type of wave function whose amplitude is large in a small region of dimensions of the order $\triangle x \triangle y \triangle z$ an negligible in the rest of space. Such a function can be constructed by superposition of a group of waves, such that they interfere constructively over only a small on region of space and produce destructive interference elsewhere. Hence a wave function of this type is called a wave-packet.

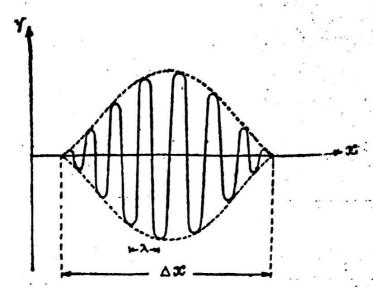


Fig. 8. Form of a typical wavepacket in one dimension.

A wave-packet, which defines the position or the momentum of a particle to a desired accuracy, can be constructed by using the superposition principle, which states that

(i) If a particle can be present in the states described by the wave functions ψ_1 and ψ_2 ; it can also be in all states described by the wave function constructed from ψ_1 and ψ_2 by the linear transformation

$$\psi = a_1 \psi_1 + a_2 \psi_2 \qquad ...(47)$$

where a_1 and a_2 are arbitrary complex numbers.

(ii) If we multiply a wavefunction by an arbitrary non-vanishing complex number, the new wavefunctions will correspond to the same state of the particle.

Let us now consider the formulation of a wave-packet. A simple harmonic wave of frequency $v=\omega/2\pi$ and wavelength $\lambda=h/p$ can be represented by the expression

$$A\cos\frac{2\pi}{\lambda}(x-vt) \qquad ...(48)$$

Here v is the velocity of motion of a point of constant phase on the wave and it is called the phase velocity of the wave.

Defining a vector \mathbf{k} (called the wave-vector or the propagation vector) having magnitude equal to $\frac{2\pi}{\lambda}$ and pointing in the direction of the wave propagation, expression (48) can be written as

$$A\cos(kx-\omega t)^* \qquad ...(49)$$

^{*}Expression of the form $A \sin(kx-\omega t)$ and $e^{\pm i(kx-\omega t)}$ also express simple harmonic waves all and these waves represent a particle of completely undetermined position travelling in the x direction with precisely known momentum and kinetic energy.

X

where $\omega = 2\pi v = 2\pi \frac{v}{\lambda} = kv$. Hence the phase velocity v is given by

$$v_{ph} = \frac{\omega}{k} \qquad \dots (50)$$

Now, a wave packet can be constructure by the superposition of the waves of the kind (49), interfering with each other in such a way that they cancel each other everywhere except in a limited region. Hence the wave-packet can be written as

$$\psi(x, t) = \int_{k_0 - \Delta k} A(k) \cos(kx - \omega t) dk. \qquad \dots (51)$$

Here $\omega(k)$ varies only in the small range of values of k. It is assumed that A(k) is negligible except when k lies in the interval $k_0 - \Delta k \leq k \leq k_0 + \Delta k$. If we assume that ω is a slowly varying function of k, we can expand $\omega(k)$ as a power series in $(k-k_0)$ retaining only the first two terms in the expansion,

$$\omega(k) = \omega_0 + \left(\frac{d\omega}{dk}\right)_0 (k - k_0), \qquad \dots (52)$$

in which the subscript zero specifies the value of the quantities at $k=k_0$. Using (52) into (51), we can write

$$\psi(x, t) = A (k_0) \int_{0}^{\infty} \cos \left[kx - \omega_0 t - (k - k_0) \left(\frac{d\omega}{dk} \right)_0 t \right] dk$$

$$= A(k_0) \int_{0}^{\infty} \cos \left[k \left\{ x - \left(\frac{d\omega}{dk} \right)_0 t \right\} - \omega_0 t + k_0 \left(\frac{d\omega}{dk} \right)_0 t \right] dk$$

$$= \frac{A(k_0)}{x - \left(\frac{d\omega}{dk} \right)_0 t} \left[\sin \left[k \left\{ x - \left(\frac{d\omega}{dk} \right)_0 t \right\} - \omega_0 t \right] + k_0 \left(\frac{d\omega}{dk} \right)_0 t \right] \right]_{k_0 - \Delta k}^{k_0 + \Delta k}$$

$$= \frac{A(k_0)}{x - \left(\frac{d\omega}{dk} \right)_0 t} \left[\sin \left[\left(k_0 + \Delta k \right) \left\{ x - \left(\frac{d\omega}{dk} \right)_0 t \right\} \right] - \omega_0 t + k_0 \left(\frac{d\omega}{dk} \right)_0 t \right] - \sin \left[\left(k_0 - \Delta k \right) \left\{ x - \left(\frac{d\omega}{dk} \right)_0 t \right\} - \omega_0 t + k_0 \left(\frac{d\omega}{dk} \right)_0 t \right] \right]$$

$$=2A(k_0)\frac{\sin\left[\left\{x-\left(\frac{d\omega}{dk}\right)_0 t\right\} \triangle k\right]}{x-\left(\frac{d\omega}{dk}\right)_0 t}.\cos(k_0x-\omega_0t) \dots (53)$$

$$\left[\text{Using, } \sin A-\sin B=2\sin\frac{A-B}{2}\cos\frac{A+B}{2}\right].$$

Equation (53) represents a wave-packet of wavelength $2 \cdot /k_0$ and frequency $\omega_0/2\pi$ with the amplitude given by the factor in front of the function $\cos(k_0x-\omega_0t)$. The form of this amplitude at t=0 is shown in fig. 9.

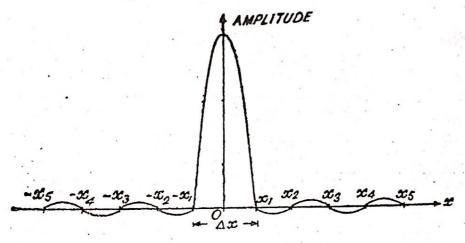


Fig. 9. Dependence of the amplitude of a wave-packet on the distance from its centre, at t=0.

The maximum value of the amplitude corresponds to the value x=0 and it is equal to 2A (k_0) $\triangle k$. For $x=x_n=n$ - $/\triangle k$ $(n=\pm 1,\pm 2,...)$, the amplitude reduces to zero. The value $\triangle x=2x_1=2\pi/\triangle k$ can be considered to be the spatial width of the wave-packet. The smaller the spread in the momentum, $p=\hbar \triangle k$, the larger the spread in space of the wave-packet. We can write from $\triangle x=2\pi/\triangle k$ that

$$\triangle x. \triangle p = h$$
 ...(54)

It is clearly the Heisenberg's uncertainty relation for the wavepacket.

The average position of the wave-packet, corresponding to the maximum of the amplitude, moves in space with a velocity

$$v_{g} = \left(\frac{d\omega}{dk}\right)_{0} \tag{55}$$

This is called the group-velocity of the wave-packet, because it is the velocity with which the group of all the waves comprising the wave-packet moves as a whole. On the other hand, as we have *

said earlier, the phase velocities are the velocities with which the individual component waves of the wave-packet moves.

So far we have said that a material particle has the wave properties and it can be represented by a wave-packet. We have also described that how to construct such a wave-packet. Now, we shall show that the velocity of the wave-packet is actually the velocity with which the material particle is moving. We know that $\mathbf{p} = \hbar \mathbf{k}$. Also, Planck's relation $E = h \nu$ can be written as $E = \hbar \omega$, because $\omega = 2\pi \nu$. From these expressions for the momentum and the energy of a particle, the group velocity of the associated wave-packet can be written as

 $v_g = \frac{d \, \sigma}{dk} = \frac{dE}{dp} \qquad ...(56)$

Quantity on the right hand side is clearly the classical Hamiltonian expression for the velocity of the particle. As an example, for a free non-relativistic particle

 $E = \frac{p^2}{2m} \; ; \; \frac{dE}{dp} = \frac{p}{m} = v.$...(57)

Thus, the velocity of a particle is identical to the group velocity of the corresponding wave-packet.

1.9. MOTION OF A WAVE-PACKET AND THE SCHROEDINGER EQUATION:

We have seen that a particle moving with a velocity v can be represented by a wave-packet, the velocity of wave-packet coincides with the velocity of the particle. Moreover, the wave-packet has large amplitude only within a small region of space and zero elsewhere, so the particle is most likely to be found where the amplitude of the wave-packet is largest. Hence we can also assign the position of the particle. Thus, we see that a wave packet completely represents a moving particles i.e., gives both, i.s velocity as well as position. In order to describe the motion of a particle, we should, therefore, set up an equation of motion for the wave-packet of the particle. It was done by E. Schroedinger in 1926, who developed a differential equation to describe the motion of the wave-packet ψ (r, t). To understand the general features of the Schroedinger theory, we begin with a very simple physical situation by considering the case of a free particle.*

^{*}The concept of the free motion of a particle is an idealisation and in reality it is completely impossible to exclude the influence of all other objects (gravitational and other fields) upon the given particle. Such an idealisation is, however necessary to simplify the theoretical description

The wave associated with a freely moving, non-relativistic particle of well defined momentum p and energy E can be represented by the complex wavefunction

$$\psi$$
 (r, t)=A exp. $\left[\frac{i}{\hbar}$ (r.p-Et) $\right]$...(58)

where $p = \hbar k$ and $E = \hbar \omega$; ω is the angular frequency of the particle wave and k is the wave-vector (or propagation vector) for the wave. The wave described by (58) is a plane wave and the planes of constant phase propagate with the phase velocity, $v_p = \omega/k$, of the wave.

The energy E and the momentum p for a free particle are

related by the equation

$$E = \frac{p^2}{2m} \cdot \dots (59)$$

Differentiating (58) with respect to time we obtain

$$\frac{\partial \psi (\mathbf{r}, t)}{\partial t} = \frac{-i}{\hbar} E \psi (\mathbf{r}, t). \qquad \dots (60)$$

If we differentiate the function ψ (r, t) twice with respect to the coordinate x, we obtain

$$\frac{\partial^2 \psi \left(\mathbf{r}, t\right)}{\partial x^2} = \frac{-p_x^2}{\hbar^2} \psi \left(\mathbf{r}, t\right) \qquad \dots (61-a)$$

and similarly for y and z, we get

$$\frac{\partial^2 \psi \left(\mathbf{r}, t\right)}{\partial y^2} = \frac{-p_y^2}{\hbar^2} \psi \left(\mathbf{r}, t\right) \qquad \dots (61-b)$$

and

$$\frac{\partial^2 \psi \left(\mathbf{r}, t \right)}{\partial z^2} = \frac{-p_z^2}{\hbar^2} \psi \left(\mathbf{r}, t \right) \qquad \dots (61-c)$$

Adding equations (61), we obtain

$$\nabla^2 \psi (\mathbf{r}, t) = -\frac{p^2}{\hbar^2} \psi (\mathbf{r}, t) \qquad \dots (62)$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian operator.

Using equations (60) and (62) into equation (59), we obtain

$$i\hbar \frac{\partial \psi (\mathbf{r}, t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi (\mathbf{r}, t)^* \qquad ...(63)$$

^{*}In order to get the Schroedinger equation we have represented a free particle by a plane wave of the form (58). We cann't start with the functions of the form $A \sin [i/\hbar (r.p-Et)]$ or $A \cos [i/\hbar (r.p-Et)]$ because the relation $E p^2/2m$ cann't be fitted for these functions.

Equation (63) is the desired Schroedinger wave equation for a free particle in the non-relativistic approximation. It is a linear differential equation and hence its solutions satisfy the principle of superposition. As we see, this equation is satisfied by all plane waves of the form (58), i.e., for all momentum p and hence is also satisfied by every linear combination of the waves. Hence, the Schroedinger equations is satisfied by a free-particle wave-packet which can be constructed by a superposition of plane-waves.

From equation (58) we have,

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = E\psi \text{ and } -i\hbar \triangle \psi(\mathbf{r}, t) = \mathbf{p} \psi(\mathbf{r}, t)...(64)$$

Thus, at least for a free particle, the energy and momentum can be represented by the following differential operators,* which, when act on the wavefuntion ψ (r. t), gives the values of the energy and the momentum of the particle.

$$E \rightarrow i\hbar \frac{\partial}{\partial t}$$
; $p \rightarrow -i\hbar \nabla$...(65)

It should be noted that these are also valid representations when the particle is not free.

We now modify the free-particle Schroedinger equation so as to include the effects of external forces that may be acting on the particle. We assume that these forces are such that they are derivable from a real potential energy function $V(\mathbf{r}, t)$, i.e.

$$\mathbf{F} = -\nabla V(\mathbf{r}, t)$$

 $\mathbf{F} = -\nabla V(\mathbf{r}, t)$ Thus equation (59) modifies to

$$E = \frac{p^2}{2m} + V(\mathbf{r}, t). \tag{66}$$

If we now use eqs. (60) and (62) into (66), we get

$$i\hbar \frac{\partial \psi (\mathbf{r}, t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi (\mathbf{r}, t) + V(\mathbf{r}, t) \psi (\mathbf{r}, t) \qquad ...(67)$$

Equation (67) is the Schroedinger wave equation that describes the motion of a particle of mass m in a force field given by Eqn.,

^{*}In quantum mechanics every dynamical quantity can be represented by an operator. When this operator acts on the wave-function, we get the original wave-function multiplied by a real constant. This real constant is the value of the dynamical quantity which a measuement will, give, if it is made on the state of the particle represented by that wave-function. In such a case, the real constant quantity is called the eigenvalue and the wavefunction as the corresponding eigenfunction of that operator. In the present example, when $i\hbar \partial/\partial t$ and $-i\hbar \nabla$ operator on the wavefunction of a particle, they, give the energy and the momentum of the particle, respectively.

 $\mathbf{F} = -\nabla V(\mathbf{r}, t)$. Since time occurs explicitly in this, we call it as the time dependent form of Schroedinger equation.

We can also write equation (67) as

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V\right) \psi = i\hbar \frac{\partial \psi}{\partial t}. \qquad ...(68)$$

Now noting that the operator $i\hbar \partial/\partial t$ operating the wavefunction ψ , gives the energy of the particle 'E', we can write (68) as

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi \qquad \dots (69)$$

As time does not occur explicitly in it, it is called the time independent form of the Schroedinger equation.

From (69), we see that the operator $(-\hbar^2/2m. \nabla^2+V)$, when operates on ψ , gives the total energy (kinetic+potential) of the particle. It is called the *Hamiltonian operator*. Thus eqn. (69) can also be written as

$$H\psi = E\psi$$
. ...(70)

This is known as the Hamiltonian form of the Schroedinger equation.

1.10. PROBABILITY INTERPRETATION OF ψ AND ITS NORMALIZATION:

The wavefunction ψ (\mathbf{r} , t), which is solution of the Schrodinger equation, is assumed to provide a quantum-mechanically complete description of the behaviour of the particle of mass m potential energy V, i.e. the result of an experiment performed upon the particle can be obtained from the wavefunction. So far, the only interpretative guide available to us is that the wavefunction be large where the particle is likely to be found and small elsewhere. This must be supplemented by other informations which obtain from the wavefuntion ψ (\mathbf{r} , t). We, therefore, need postulates, which can allow us to deduce the result of an experiment from the knowledge of ψ (\mathbf{r} , t).

The fundamental postulate in this regard was given by Max Born, which states that the quantity $\psi^* \psi = |\psi|^2$ is proportional to the probability density, $P(\mathbf{r}, t)$, for finding a particle in the state $\psi(\mathbf{r}, t)$. Thus, the probability of finding the particle in a volume element $d^3r = dxdydz$ about the point \mathbf{r} is proportional to $\psi^* \psi d^3r$, i.e.

$$P(\mathbf{r},t) d^3r \propto \psi^* \psi d^3r. \tag{71}$$

If we make an investigation for finding the particle in the entire space, then the particle is certainly to be found somewhere in the space. Therefore, the total probability of finding the particle in the entire space must be equal to unity; i.e.

$$\int P(\mathbf{r}, t) d^3r = 1.$$
 ...(72)

The proportionality between $P(\mathbf{r}, t)$ and $\psi^*\psi$ in eqn. (71) introduces a constant which can be determined from eqn (72). From eqn (71), we get:—

$$1 = \int P(\mathbf{r}, t) d^3r = C \int \psi^* \psi d^3r. \qquad ...(73)$$
all space all space

Here, C is the constant of proportionality and it is given by:

$$C = \frac{1}{\int \psi^{\pm} \psi \ d^3r} \qquad \dots (74)$$
all space

$$P(\mathbf{r}, t) = \frac{\psi^* \psi}{\int \psi^* \psi \ d^3 r} \qquad \dots (75)$$

From eqn. (75), it is clear that $P(\mathbf{r}, t)$ remains unchanged if $\psi(\mathbf{r}, t)$ is multiplied by any constant factor. From the superposition principle, this does not change the fact that ψ is a solution of the Schroedinger eqn. Hence, two wave-functions differing only by a constant factor describe identical physical systems. If we introduce a factor which makes the denominator on the right-hand of eqn. (75) equal to unity, then $P(\mathbf{r}, t) = \psi_1 * \psi_1$, where

$$\psi_1 = \frac{1}{\sqrt{(N)}} \psi ; N = \int \psi^* \psi \ d^3 r. \qquad \dots (76)$$
all space

The function ψ_1 , defined in this way, satisfies the equation

$$\int \psi_1^* \psi_1 \ d^3r = 1 \qquad \dots (77)$$
all space

and it is said to be normalized.

The normalization constant of ψ must be independent of time so that the wavefunction ψ_1 may satisfy the Schroedinger equation.

We shall now show that the constant N is actually independent of time for every wave function ψ of the Schrödinger's equation—

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial \psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V \psi(\mathbf{r}, t) \qquad ...(78)$$

Taking the complex conjugate of eqn. (78), we get

$$-i\hbar \frac{\partial \psi^* (\mathbf{r}, t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi^*(\mathbf{r}, t) + V \psi^*(\mathbf{r}, t), \qquad ...(79)$$

Now, from eqn. (76), we have that

$$\frac{dN}{dt} = \int \left(\psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \psi \right) d^3r. \qquad ...(80)$$
all space

Putting the value of $\partial \psi / \partial t$ and $\partial \psi^* / \partial t$ into (80) from eqns. (78) and (79), we obtain

$$\frac{dN}{dt} = \frac{i\hbar}{2m} \int (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*) d^3r. \qquad ...(81)$$
all space

Using Green's theorem, this integral can be transformed into a surface integral as:—

$$\frac{dN}{dt} = \frac{i\hbar}{2m} \int (\psi^* \nabla \psi - \psi \nabla \psi^*) \cdot \hat{n} \, ds \qquad \dots (82)$$

where S is the surface enclosing the volume of integration and n is the unit vector normal to the surface element ds. Now the wavefunction ψ should vanish at large distances in order to define the position of the particle. Hence the surface integral in eqn. (82) approaches zero as the surface of integration recedes to infinity.

$$\frac{dN}{dt} = 0,$$

and, consequently, the normalization constant is independent of time.

Another interpretation of ψ may be given by considering a single region of space that contains a large number of particles each of which is described by the same wavefunction ψ . Then the quantity $|\psi|^2$ represents the average number of particles which will be found in unit volume at the point \mathbf{r} , when an experiment is made to detect them. Hence, the absolute square of the weve function represents the average particle density at \mathbf{r} . If the particles are charged, the product of the charge of a particle and $|\psi|^2$ ives the charge density.

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1.11. STATIONARY-STATE SOLUTIONS OF THE SCHROE-DINGER EQUATION:

If the probability distribution $\psi^*\psi$, for the state of the system described by the wavefunction ψ (\mathbf{r} , t), is independent of time, then the state of the system is said to be a stationary state. In order to find out the stationary state solutions of the Schroedinger's equation,

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V\right) \psi = i\hbar \frac{\partial \psi}{\partial t}, \qquad \dots (83)$$

we apply the method of separation of variables. If the potential energy V is assumed to be independent of time and depends on position only, then ψ may be expressed in the form

$$\psi = \phi(\mathbf{r}) \chi(t) \qquad \dots (84)$$

Substituting this value of ψ in eqn. (83), we get

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V\right) \phi(\mathbf{r}) \chi(t) = t\hbar \frac{\partial \chi(t)}{\partial t} \phi(\mathbf{r})$$

Dividing throughout by $\phi(\mathbf{r}) \chi(t)$, we can write this equation as

$$\frac{1}{\phi(\mathbf{r})} \left(\frac{-\hbar^2}{2m} \nabla^2 \phi(\mathbf{r}) + V(\mathbf{r}) \phi(\mathbf{r}) \right) = \frac{i\hbar}{\chi(t)} \frac{\partial \chi(t)}{\partial t}...(85)$$

In Eqn. (85), left hand side is independent of time, while the right hand side is independent of the coordinate \mathbf{r} Therefore, this equation will be satisfied if each side of it is equal to a constant E (say). Hence we write

$$\frac{1}{\phi(\mathbf{r})} \left(\frac{-h^2}{2m} \nabla^2 \phi(\mathbf{r}) + V(\mathbf{r}) \phi(\mathbf{r}) \right) = E \text{ and } \frac{i\hbar}{\chi(t)} \frac{\partial \chi(t)}{\partial t} = E \quad ...(86)$$

or
$$\nabla^2 b + \frac{\hbar^2}{2m} (E \ V) \phi = 0$$
 and $\frac{\partial \chi(t)}{\partial t} = -\frac{iE}{\psi} \chi(t)$(87)

Solution of the 2nd of the equations (87) may be written as

$$\chi(t) = e^{-iEt/\hbar} \qquad \dots (88)$$

Comparing this equation with that for a plane weve we see that the dimensions of E must be that of the energy Thus we can say that the constant E designates the energy of the particle which is described by this solution of Schrodinger equation. With this value of χ (t) eqn. (84) becomes

$$\psi(\mathbf{r}, t) = \phi(\mathbf{r}) e^{-iEt/\hbar} \qquad ... (89)$$

For a particle confined to a finite region, the function ϕ (r) will be single valued, continuous and finite*, only for certain definite values of energy E. These allowed values of E are called the eigen values. Corresponding to each allowed value of E, there will

be one function ψ , referred as the eigen function. Thus we have finitely many solutions of the Schroedinger equation for timeindependent potential energy V (r). These can be written as:—

$$\phi_1$$
 (r) $e^{-i E_1 t/\hbar}$, ϕ_2 (r) $e^{-i E_2 t/\hbar}$,, ϕ_n (r) $e^{-i E_n t/\hbar}$...(90)

For each of these solutions we see that $\psi^*\psi$ is independent of time and hence these are the stationary state solutions of the Schrödinger's Eqn.

1.12. PROBABILITY CURRENT DENSITY

The time dependent Schroedinger's equation is given by

$$\frac{-\hbar^2}{2m} \nabla^2 \psi + V \psi = i\hbar \frac{\partial \psi}{\partial t} \qquad ...(91)$$

Taking its complex conjugate, we get

$$\frac{-\hbar^2}{2m} \cdot \nabla^2 \psi^* + V \psi^* = -i\hbar \frac{\partial \psi^*}{\partial t} \qquad \dots (92)$$

Multiplying equation (91) by ψ^* and equation (92) by ψ we get

$$\frac{-\hbar^2}{2m} \psi^* \nabla^2 \psi + V \psi^* \psi = i\hbar \psi^* \frac{\partial \psi}{\partial t} \qquad \dots (93)$$

and

$$\frac{-\hbar^2}{2m} \psi \nabla^2 \psi^* + V \psi^* \psi = -i\hbar \psi \frac{\partial \psi^*}{\partial t} \qquad ...(94)$$

Subtracting equation (94) from (93), we obtain

$$\frac{-\hbar^{2}}{2m} (\psi^{*} \nabla^{*} \psi - \psi \nabla^{2} \psi^{*}) = i \hbar \left(\psi^{*} \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^{*}}{\partial t} \right)$$
or
$$\frac{\partial}{\partial t} (\psi^{*} \psi) + \frac{\hbar}{2im} \nabla \cdot (\psi^{*} \nabla \psi - \psi \nabla \psi^{*}) = 0 \qquad \dots (95)$$

Since the Schrodinger's equation is a linear partial differential equation of second order in space coordinates, its solution $\psi(\mathbf{r}, t)$ should be continuous and should have continuous first derivative with respect to the space coordina es so that the equation can be integrated to get the wavefunction. Further, the probability of finding the particle in a state represented by wavefunction ψ; given by ψ*ψ; should be unique. Hence the Schrodinger's wavefunction Should also be single valued. Furthermore, the probability $\psi^*\psi dr^*$ should be finite and hence the wavefunction should be finit everywhere and should

vanish at infinite distances.

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This equation is analogous to the well-known equation of continuity in hydrodynamics, i.e.,

$$\frac{\partial \rho}{\partial t} + \nabla . \mathbf{S} = 0 \qquad \dots (96)$$

in which $\rho = \psi^* \psi$ is the probability density, and S, the probability current density is given by,

$$S = \frac{\hbar}{2im} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) = \text{Real part of} \left(\psi^* \frac{\hbar}{im} \nabla \psi \right). \quad ...(97)$$

This equation makes more plausible the identification of $-i\hbar \nabla$ as the momentum operator even in the presence of forces; then \hbar/im . ∇ is the velocity operator and $\mathbf{S} = Re$. $\rho \mathbf{v} = \rho \mathbf{v}$ is the current of probability density.

In hydrodynamics, eqn. (96) corresponds to the conservation of mass of the fluid; i.e., a change in the total amount of fluid contained within any small fixed volume element is accounted for by flow through the surface of the volume element. Therefore, in quantum mechanics, equation (96) tells that a decrease of the probability of finding a particle within a volume V can be described in terms of an outward flow of probability current S through the surface of V. The decrease of probability arises due to the change of ψ with time.

It should be noted that S cannot be measured directly like $\rho = \psi^* \psi$. This is due to the fact that the measurement of S will require simultaneous measurements of the position and the velocity which is not possible due to uncertainty relation.

1.13. EXPECTATION VALUES OF DYNAMICAL QUANTITIES:

It has been seen that $\psi^*\psi$ gives the probability density for finding the position of the particle. We can, therefore, calculate the "average" or "expected" value of the position of the particle. It; can be written as:

$$\langle \mathbf{r} \rangle = \frac{\int \mathbf{r} \, \psi^*(\mathbf{r}, t) \, \psi(\mathbf{r}, t) \, d^3r}{\int \psi^*(\mathbf{r}, t) \, \psi(\mathbf{r}, t) \, d^3r} \qquad \dots (98)$$

Thus, the average value of position of the particle is the mathematical average for the result of a measurement performed on the particle in the state ψ (r, t).

If ψ (r, t) is normalized, we can write eqn. (98) as:

$$\langle \mathbf{r} \rangle = \int \psi^* (\mathbf{r}, t) \mathbf{r} \psi (\mathbf{r}, t) d^3r \qquad ...(99)$$

This is equivalent to the following three expressions,

$$\langle x \rangle = \int \psi^* (\mathbf{r}, t) x \psi (\mathbf{r}, t) d^3r$$

$$\langle y \rangle = \int \psi^* (\mathbf{r}, t) y \psi (\mathbf{r}, t) d^3r \qquad \dots (100)$$

$$\langle z \rangle = \int \psi^* (\mathbf{r}, t) z \psi (\mathbf{r}, t) d^3r$$

In general, the expectation value of any function $f(\mathbf{r})$ of the coordinates of the particle would be given by,

$$\langle f(\mathbf{r}) \rangle = \int \psi^*(\mathbf{r}, t) f(\mathbf{r}) \psi(\mathbf{r}, t) d^3r.$$
 ...(101)

The expectation value of the potential energy, which is also the function of position, is written as

$$\langle V \rangle = \int \psi^* (\mathbf{r}, t) V \psi (\mathbf{r}, t) d^3r \qquad ...(102)$$

So far we have considered the expectation values of the quantities which depend upon the position coordinates only. In order to define the expectation values of other quantities which are of dynamical interest, such as momentum and energy, we start with the reasonable requirement that

$$\langle E \rangle = \left\langle \frac{p^2}{2m} \right\rangle + \langle V \rangle.$$
 ...(103)

Replacing **p** and *E* by their differential operators, $-i\hbar \nabla$ and $i\hbar \frac{\partial}{\partial t}$; respectively, we can write (103) as:

$$\langle i\hbar \frac{\partial}{\partial t} \rangle = \langle -\frac{\hbar^2}{2m} \nabla^2 \rangle + \langle V \rangle \qquad \dots (104)$$

Now, multiplying the Schroedinger's equation by ψ^* and integrating it, we get:

$$\int \psi^* i \hbar \frac{\partial \psi}{\partial t} d^3r = \int \psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \psi d^3r + \int \psi^* V \psi d^3r \dots (105)$$

The last term on the right hand side of eqn. (105) is simply $\langle V \rangle$; thus Eqns. (104) and (105) would be consistent, only if, the expectation value is defined in the general case as the operator acting on ψ and multiplied on the left by ψ^* and then integrated. Thus we obtain

$$\langle E \rangle = \int \psi^* i \hbar \frac{\partial \psi}{\partial t} d^3r$$
 ...(106)

and
$$\langle \mathbf{p} \rangle = \int \psi^* (-i\hbar) \nabla \psi d^3r \qquad \dots (107)$$

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Eq. (107) is equivalent to the following three equations

$$\langle p_{z} \rangle = -i \hbar \int \psi^{*} \frac{\partial \psi}{\partial x} d^{3}r$$

$$\langle p_{y} \rangle = -i \hbar \int \psi^{*} \frac{\partial \psi}{\partial y} d^{3}r \qquad ...(108)$$

$$\langle p_{z} \rangle = -i \hbar \int \psi^{*} \frac{\partial \psi}{\partial z} d^{3}r.$$

1.14 EHRENFEST THEOREM; CORRESPONDENCE PRIN-CIPLE:

It was discussed in the beginning of this chapter that the laws of classical mechanics were found inadequate to describe the observed behaviour of the microscopic systems. On the other hand, the classical theory is well established on the basis of experimental observations for the systems of macroscopic size. Thus, we can think that the quantum theory will give the results identical with those of the classical theory if the masses and dimensions of the system under consideration are made to approach the macroscopic size. This fundamental idea was first stated by Bohr and it is known as Bohr's Correspondence Principle. Later on, it was shown by Ehrenfest that if we ignore the finite size and Internal structure of the wave packet corresponding to a moving particle, and consider only the average motion of the wavepacket, it indeed coincides with the classical motion of the particle. Thus, the Bohr's correspondence principle was actually demonstrated by Ehrenfest by showing that the newton's laws of motion, in the form

(i)
$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{m}$$
, (ii) $\frac{d\mathbf{p}}{dt} = -\nabla V$...(109)

are satisfied exactly by the average motion of a wave-packet $\psi(\mathbf{r}, t)$ which is a solution of the Schroedinger's equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad ...(110)$$

To show it, we first consider the average expectation value of x for the packet,

$$\langle x \rangle = \int \psi^* x \, \psi \, d^3 r. \qquad \dots (111)$$

Differentiating it w.r.t. time, we obtain

$$\frac{d\langle x\rangle}{dt} = \int \left[\frac{\partial \psi^*}{\partial t} x \psi + \psi^* \overline{x} \frac{\partial \psi}{\partial t}\right] d^3r. \qquad \dots (112)$$

Substituting the values of $\partial \psi / \partial t$ and $\partial \psi^* / \partial t$ from equation (110) and its complex conjugate; respectively, we can write (112) as

$$\frac{d\langle x\rangle}{dt} = \frac{1}{i\hbar} \left[\int \psi^* x \left(\frac{-\hbar^2}{2m} \nabla^2 \psi + V \psi \right) \right) d^3r
- \int \left(\frac{-\hbar^2}{2m} \nabla^2 \psi^* + V \psi^* \right) x \psi d^3r \right]
= \frac{i\hbar}{2m} \int \left[\psi^* x \nabla^2 \psi - (\nabla^2 \psi^*) x \psi \right] d^3r \qquad \dots (113)$$

Now,
$$\int (\nabla^2 \psi^*) x \psi d^3 r = \int \nabla \cdot (x \psi \nabla \psi^*) d^3 r - \int (\nabla \psi^*) \cdot \nabla (x \psi) d^3 r$$
...(114)

The first integral on the right hand side can be transformed into a surface integral by using the Gauss's theorem,

$$\int \nabla \cdot (x\psi \nabla \psi^*) \ d^3 r = \int_s (x\psi \nabla \psi^*)_n \ ds$$

where the subscript 'n' denotes the normal component of the vec-The surface integral over the surface tor inside the parenthesis at infinity vanishes because the wave-paket ψ vanishes at infinity. Consequently,

$$\int (\nabla^2 \psi^*) x \psi d^3 r = -\int (\nabla \psi^*) \cdot \nabla (x \psi) d^3 r$$

$$= -\left[\int \nabla \cdot (\psi^* \nabla (x \psi)) d^3 r - \int \psi^* \nabla^2 (x \psi) d^3 r \right]$$

Once again, the first integral on the R.H.S. can be transformed to a surface integral which would vanish. Thus

$$\int (\nabla^2 \psi^*) \ x \psi d^3 r = \int \psi^* \nabla^2 (x \psi) \ d^3 r$$

Substituting this result in Eqn. (113), we obtain

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m} \int \left[\psi^* \left\{ x^2 \nabla^2 \psi - \nabla^2 \left(x \psi \right) \right\} \right] d^3r. \qquad \dots (115)$$

Now,
$$x \nabla^2 \psi - \nabla^2 (x\psi) = x \nabla^2 \psi - \nabla \cdot \nabla (x\psi)$$

$$= x \nabla^2 \psi - \nabla \cdot \{(\nabla x) \psi + x \nabla \psi\}$$

$$= x \nabla^2 \psi - (\nabla x) \cdot (\nabla \psi) - (\nabla^2 x) \psi$$

$$- (\nabla x) \cdot (\nabla \psi) - x \nabla^2 \psi$$

$$= -2 (\nabla x) \cdot (\nabla \psi) \qquad \{\because (\nabla^2 x) = 0\}$$

$$= -2 \frac{\partial \psi}{\partial x} \cdot \dots (116)$$

$$\frac{d\langle x\rangle}{dt} = \frac{-i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} d^3r = \frac{1}{m} \langle p_x \rangle \qquad \dots (117)$$

Similarly, we can prove that

$$\frac{d\langle y\rangle}{dt} = \frac{1}{m}\langle p_y\rangle \text{ and } \frac{d\langle z\rangle}{dt} = \frac{1}{m}\langle p_z\rangle.$$
 ...(118)

Hence, from eqns. (117) and (118), we have

$$\frac{d\langle \mathbf{r} \rangle}{dt} = \frac{1}{m} \langle \mathbf{p} \rangle \qquad \dots (119)$$

Now, the time rate of change of $\langle p_x \rangle$ may be written as,

$$\frac{d \langle p_x \rangle}{dt} = \frac{d}{dt} \int \psi^* \left(-i\hbar \right) \frac{\partial \psi}{\partial x} d^3r$$

$$= -i\hbar \int \left[\frac{\partial \psi^*}{\partial t} \cdot \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial}{\partial t} \left(\frac{\partial \psi}{\partial x} \right) \right] d^3r$$

$$= -i\hbar \int \left[\frac{\partial \psi^*}{\partial t} \cdot \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial t} \right) \right] d^3r$$

$$= \left[\int \left(\frac{-\hbar^2}{2m} \nabla^2 \psi^* + V \psi^* \right) \frac{\partial \psi}{\partial x} d^3r$$

$$- \int \psi^* \frac{\partial}{\partial x} \left(\frac{-\hbar^2}{2m} \nabla^2 \psi + V \psi \right) d^3r \right]$$

[Using Schroedinger's equation and its complex conjugate]

$$= \frac{-\hbar^2}{2m} \int \left[\nabla^2 \psi^* \frac{\partial \psi}{\partial x} - \psi^* \nabla^2 \frac{\partial \psi}{\partial x} \right] d^3r - \int \psi^* \left(\frac{\partial V}{\partial x} \right) \psi \ d^3r$$
 ...(120)

Applying Green's theorem, we can write the first term on the right hand side as,

$$\iint \left[\nabla^2 \psi^* \frac{\partial \psi}{\partial x} - \psi^* \nabla^2 \frac{\partial \psi}{\partial x} \right] d^3 r = \iint_{S} \left[\nabla \psi \frac{\partial \psi}{\partial x} - \psi^* \nabla \frac{\partial \psi}{\partial x} \right]_n ds$$

=0, for the surface at infinity

$$\therefore \frac{d\langle p_x \rangle}{dt} = -\int \psi^* \left(\frac{\partial V}{\partial x}\right) \psi d^3r = \left\langle -\frac{\partial V}{\partial x}\right\rangle \qquad \dots (121)$$

Similarly, we can prove that,

$$\frac{d\langle p_y \rangle}{dt} = \left\langle -\frac{\partial V}{\partial y} \right\rangle \text{ and } \frac{d\langle p_z \rangle}{dt} = \left\langle -\frac{\partial V}{\partial z} \right\rangle. \quad \dots (122)$$

From equations (121) and (122), we can write that

$$\frac{d\langle \mathbf{p} \rangle}{dt} = \langle -\nabla V \rangle. \tag{123}$$

Equations (119) and (123) are analogous to equations (109) of classical physics. This proves Ehrenfest's theorem.

1·15. EXACT STATEMENT AND PROOF OF UNCERTAINTY PRINCIPLE FOR WAVE-PACKET:

Before giving the proof and the exact statement of the Heisen-

berg's uncertainty principle, we first define the uncertainty in the measurement of the position and the momentum. From the analogy of standard deviation in statistics, we may define the uncertainties $\triangle x$ and $\triangle p_x$ in the position and the momentum as the mean square deviations of position and the momentum from the averages $\langle x \rangle$ and $\langle p_x \rangle$ as:—

$$(\triangle x)^2 = \int \psi^* (x - \langle x \rangle)^2 \psi d^3r = \langle \{x - \langle x \rangle\}^2 \rangle \qquad \dots (124)$$

and $(\triangle p_x)^2 = \int \psi^* (p_x - \langle p_x \rangle)^2 \psi d^3r = \langle \{p_x - \langle p_x \rangle\}^2 \rangle$, ...(125)

where, $\langle x \rangle = \int \psi^* x \psi d^3r$ and $\langle p_x \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} d^3r$.

First we prove the uncertainty principle for the case of a wave packet for which $\langle x \rangle = \langle p_x \rangle = 0$, so that ...(126)

 $(\triangle x)^2 = \langle x^2 \rangle$ and $(\triangle p_x)^2 = \langle p_x^2 \rangle$...(12)

Let us now consider the integral,

$$i\hbar \int \frac{d\psi^*}{dx} x\psi \ d^3r = i\hbar \int \psi^* x\psi \ d^3r - i\hbar \int \psi^* \frac{d(x\psi)}{dx} \ d^3r$$

$$= i\hbar \langle x \rangle - i\hbar \int \psi^* \frac{d\psi}{dx} x \ d^3r - i\hbar \int \psi^* \psi \ d^3r$$

$$= -i\hbar \int \psi^* \frac{d\psi}{dx} x \ d^3r - i\hbar$$

$$\{ \because \langle x \rangle = 0 \text{ and } \int \psi^* \psi \ d^3r = 1 \}$$

or
$$i\hbar \int \frac{d\psi^*}{dx} x \psi \, d^3r + i\hbar \int \psi^* \frac{d\psi}{dx} x \, d^3r = -i\hbar$$
or
$$2i \operatorname{Im} \cdot i\hbar \int \frac{d\psi^*}{dx} x \psi \, d^3r = -i\hbar \qquad \dots (127)$$

Taking modulus of both sides and then squaring we get

$$4 \left| Im.i\hbar \int \frac{d\psi^*}{dx} x\psi d^3r \right|^2 = \hbar^2 \qquad \dots (128)$$

Since the magnitude of the imaginary part of a complex number cannot exceed the modulus of the number itself, we can write from eqn (128) that

$$4 \left| i\hbar \int \frac{d\psi^*}{dx} x\psi d^3r \right|^2, \geqslant \hbar^2 \qquad \dots (129)$$

According to Schwarz inequality,

$$\left| \int f * g \ d^3r \right|^2 \leqslant \int f * f \ d^3r \int g * g \ d^3r. \qquad \dots (130)$$

If we take
$$f *= i\hbar \frac{d\psi^*}{dx}$$
 and $g = x\psi$, then eqn. (130) gives
$$\left| i\hbar \int \frac{d\psi^*}{dx} x\psi \ d^3r \right|^2 \leqslant \int i\hbar \frac{d\psi^*}{dx} \cdot -i\hbar \frac{d\psi}{dx} \ d^3r. \int x\psi^* x\psi \ d^3r$$

$$= \int \left| -i\hbar \frac{d\psi}{dx} \right|^2 \ d^3r. \int x^2 |\psi|^2 \ d^3r$$

$$= \langle p^2_x \rangle \cdot \langle x^2 \rangle \qquad \dots (131)$$

Using inequality (131) into eqn. (129), we get

or
$$(\triangle x)^2 \cdot (\triangle p_x)^2 \geqslant \frac{\hbar^2}{4} \{\text{using eqn. (126)}\}$$
or $\triangle x \cdot \triangle p_x \geqslant \frac{\hbar}{2}$...(132)

This is the exact statement of Heisenberg's uncertainty principle. But now we should show that the relation (132) also holds good for the wave-packets for which $\langle x \rangle$ and $\langle p_x \rangle$ are nonzero. For it, let us define $\alpha = x - \langle x \rangle$ and $\beta = p_x - \langle p_x \rangle$, then $\langle \alpha \rangle = \langle x - \langle x \rangle = \langle x \rangle - \langle x \rangle = 0$ and similarly $\langle \beta \rangle = 0$.

Since $\langle \alpha \rangle = \langle \beta \rangle = 0$, therefore, as above we can reach at the equation.

or
$$\langle \{x-\langle x\rangle\}^2\rangle \langle \{p_x-\langle p_x\rangle\}^2\rangle \geqslant \frac{\hbar^2}{4}$$
.
or $(\triangle x)^2 (\triangle p_x)^2 \geqslant \frac{\hbar^2}{4}$ {using eqns. (124) and (125)}
 $\therefore (\triangle x) (\triangle p_x) \geqslant \frac{\hbar}{2}$.

This completes the proof.

PROBLEMS

Problem 1. What is the energy of gamma photon having a wavelength of one \mathring{A} . Given Planck's constant $h=6.62\times10^{-27}$ ergs-sec.

Sol. The velocity of gamma photons is equal to that of the light, i.e., 3×10^{10} cms/sec. Here, we are given that the wavelength of the gamma photon, $\lambda = 1 \text{ Å} = 10^{-8}$ cm. Therefore, the frequency of the photon is given by—

$$v = \frac{3 \times 10^{10}}{10^{-8}} = 3 \times 10^{18}$$
 cycles per sec.

From the Planck's law, E=hv, the energy of the photon will be.

$$E=6.62\times10^{-27}\times3\times10^{18} \text{ ergs}$$

$$=\frac{6.62\times10^{-27}\times3\times10^{18}}{1.6\times10^{-12}}=1.24\times10^{4} \text{ eV}.$$

Problem 2. The work function of zinc is 3.6 eV. What is the maximum energy of the photoelectrons ejected by ultraviolet light of wavelength 3000 Å.

Sol. From Einstein's photo-electric equation, the maximum energy of the photo-electrons is given by

$$\frac{1}{2}mv^2 = h_V - W_0.$$
 ...(i)

Here, the work function $W_0 = 3.6 \text{ eV} = 3.6 \times 1.6 \times 10^{-12} \text{ ergs.}$ Frequency of the U.V. light of wave-length 3000 Å is given

$$v = \frac{c}{\lambda} = \frac{3 \times 10^{10}}{3000 \times 10^{-8}} = 10^{15}$$
 cycles per second.

$$h_{V} = 6.62 \times 10^{-27} \times 10^{15} = 6.62 \times 10^{-12} \text{ ergs.} \qquad \dots \text{(ii)}$$

Hence, $\frac{1}{2}mv^2 = 6.62 \times 10^{-12} - 3.6 \times 1.6 \times 10^{-12} = 86 \times 10^{-12}$ ergs.

Problem 3. The photoelectric threshold for a certain metal is 3600 Å. Calculate the maximum energy of the ejected photoelectrons by a radiation of 2000 Å.

Sol. Here,
$$\lambda_0 = 3600 \text{ Å} = 36 \times 10^{-6} \text{ cm.}$$

$$\nu_0 = \frac{c}{\lambda_0} = \frac{3 \times 10^{10}}{36 \times 10^{-6}} = \frac{1}{12} \times 10^{16} \text{ cycles/sec.}$$

$$W_0 = h\nu_0 = \frac{6 \cdot 625 \times 10^{-27} \times 10^{16}}{12} = 0.5521 \times 10^{-11} \text{ ergs}$$

$$= \frac{0.5521 \times 10^{-11}}{1.6 \times 10^{-12}} = 3.45 \text{ eV.}$$

Now, the wavelength of the incident light, $\lambda = 2000 \text{ Å}$ = $2 \times 10^{-5} \text{ cm}$.

$$v = \frac{c}{\lambda} = \frac{3 \times 10^{10}}{2 \times 10^{-5}} = 1.5 \times 10^{15} \text{ cycles/sec.}$$

$$hv = \frac{6.625 \times 10^{-27} \times 1.5 \times 10^{15}}{1.6 \times 10^{-12}} = 6.21 \text{ eV.}$$

From Einstein's photo-electric equation, maximum energy is given by, $\frac{1}{2}mv^2 = hv - W_0 = 6.21 - 3.45 = 2.76 \text{ eV}.$

Problem 4. According to classical theory, a charge e, subjected to an acceleration $\ddot{\mathbf{r}}$, radiates energy at the rate

$$\frac{dE}{dt} = -\frac{2}{3} \frac{e^2 (\ddot{\mathbf{r}})^2}{c^3} \qquad ...(i)$$

Considering a classical model of hydrogen atom, with an electron moving in a circular orbit about the nucleus, find the time during which the radius of the atom would shrink to half. (Initial radius $r_0=0.5\times10^{-8}$ cm).

Sol. The total energy of the hydrogen atom is given by $E = -\frac{e^2}{2r}$, where r is the radius of the atom. The acceleration is $\ddot{\mathbf{r}} = \frac{v^2}{r} = \frac{e^2}{mr^2}$, where v is the velocity and m is the mass of the electron.

The equation for the radiation rate may now be written as

$$\frac{dE}{dt} = \frac{e^2}{2r^2} \frac{dr}{dt} = -\frac{2}{3} \frac{e^2}{c^3} \left(\frac{e^2}{mr^2}\right)^2$$

$$\therefore dt = -\frac{3}{4} \frac{m^2 c^3}{e^4} r^2$$

The time t for the radius to shrink from r_0 to $\frac{r_0}{2}$ is, then

$$t = -\frac{3}{4} \frac{m^2 c^3}{e^4} \int_{r_0}^{r_0/2} r^2 dr = \frac{7}{32} \frac{m^2 c^3 r_0^3}{e^4} \approx 1.4 \times 10^{-11} \text{ sec.}$$

Problem 5. A photon of energy 1.02 Mev is scattered through 90° by a free electron. Calculate the energy of photon and electron after interaction.

Sol. Change in wave-length of the photon is given by

$$\Delta \lambda = \frac{h}{m_0 c} (1 - \cos \phi) = \frac{6.62 \times 10^{-27}}{9.1 \times 10^{-28} \times 3 \times 10^{10}} (1 - \cos 90^\circ)$$

$$= 2.42 \times 10^{-10}$$

.. Change in frequency of photon, $\Delta v = \frac{c}{\Delta \lambda} = \frac{3 \times 10^{10}}{2.42 \times 10^{-10}}$ cyces/sec.

Change in energy of photon, $\triangle E = h$. $\triangle v = 0.51$ Mev.

This energy is transferred to the free electron.

:. Kinetic energy of electron after interaction=0.51 Mev and remaining energy of photon after interaction

$$=1.02-0.51=0.51$$
 Mev.

Problem 6. In an experiment on the diffraction of electrons by G. P. Thomson method, the diameter of the first order ring at an applied voltage of 10,000 volts was 1.82 cm. Calculate the spacing of the reflecting planes of the foil. (For simplicity, neglect the relativity correction.)

Planck's constant= 6.624×10^{-27} erg sec. Mass of the electron= 9.113×10^{-28} gm. Electron Charge = 4802×10^{-10} e.s.u.

Distance between the foil and the screen=2.5 cm.

Sol. The wavelength of an electron, accelerated through a potential difference of V volts is given by

$$\lambda = \sqrt{\left(\frac{150}{V}\right)} \mathring{A}$$

V=10,000 volts.

$$\lambda = \sqrt{\frac{150}{10,000}} \, \mathring{A} = 0.1227 \times 10^{-8} \, \text{cm}$$

The radius of the first order ring will be,

$$\dot{r} = \frac{1.82}{2} = 0.91$$
 cm.

The distance of the foil from the screen, D=2.5 cm.

Hence the spacing of the reflecting planes is given by
$$d = \frac{Dn\lambda}{r} = \frac{2.5 \times 1 \times 0.1227 \times 10^{-8}}{0.91} = 0.3363 \text{ Å.}$$

Problem 7. A particle of mass 0.5 MeV/c2 has kinetic energy 100 eV. Calculate its de-Broglie wave-length.

Sol. Mass of the particle =
$$\frac{0.5MeV}{c^2}$$

= $\frac{0.5 \times 10^6 \times 1.6 \times 10^{-12}}{(3 \times 10^{10})^2}$ gms.
= $\frac{80}{9} \times 10^{-28}$ gms.

Now, the kinetic energy, $\frac{1}{2} mv^2 = 100 eV$. $=100\times1.6\times10^{-12}$ ergs.

$$m^2v^2 = 2 \times 100 \times 1.6 \times 10^{-12} \times \frac{80}{9} \times 10^{-28}$$

or

$$mv \cong \frac{160}{3} \times 10^{-20}$$

Hence, the de-Broglie wave-length
$$\lambda$$
 is given by
$$\lambda = \frac{h}{mv} = \frac{6.625 \times 10^{-27} \times 3}{160 \times 10^{-20}} = 1.243 \text{ Å.}$$

Problem 8. Determine the wave-length associated with an electron having kinetic energy 1 MeV.

Sol. Since the energy 1 Mev is comparable with the rest mass energy of the electron, we must use the relativistic equation:

$$mc^{2} = m_{0}c^{2} + V.E. = 0.512 + 1 = 1.512, MeV$$

$$\therefore m = \frac{1.512 \times 1.6 \times 10^{-6}}{(3 \times 10^{10})^{2}} = 3.18 \times 10^{-17} \text{ gm}.$$

Putting this value of m in the relation, $m = \frac{m_0}{\sqrt{\left(1 - \frac{v^2}{c^2}\right)}}$

we get:

$$3.18 \times 12^{-27} = \frac{9.11 \times 10^{-28}}{\sqrt{\left\{1 - \frac{v^2}{(3 \times 10^{10})^2}\right\}}}$$

Solving it, we obtain $v=2.87\times10^{10}$ cm/sec.

$$\lambda = \frac{h}{mv} = \frac{6.625 \times 10^{-27}}{3.18 \times 10^{-27} \times 2.87 \times 10^{10}} = 0.00276 \text{ Å}.$$

Problem 9. A beam of mono-energetic neutrons corresponding to 27°C is allowed to fall on a crystal. A first order reflection is observed at a glancing angle 30°. Calculate the interplaner spacing of the crystal.

Sol. The energy of the neutrons at temperature $T^{\circ}K$ is given by, E=kT ergs, where $k=1.38\times10^{-10}$ erg/°k is Boltzman's constant. Here,

$$T = 273 + 27 = 300^{\circ} K$$

$$\therefore E = 1.38 \times 10^{-16} \times 300 = 4.14 \times 10^{-14} \text{ ergs.}$$
Thus, $\frac{1}{2}Mv^2 = 4.14 \times 10^{-14}$
or
$$Mv = \sqrt{(2 \times 4.14 \times 10^{-14} \times M)}$$

$$= \sqrt{(2 \times 4.14 \times 10^{-14} \times 1.67 \times 10^{-24})}$$

$$\therefore \lambda = \frac{h}{mv} = 1.78 \times 10^{-8} \text{ cm.}$$

Using this value of λ in the Bragg's law, $2d \sin \theta = n\lambda$,

$$2d \sin 30^{\circ} = 1 \times 1.78 \times 10^{-8}$$

 $d = 1.78 \text{ Å}.$

Problem 10. What is the de Broglie wavelength of a neutron with a velocity equal to the most probable velocity of a Maxwell distribution corresponding to an absolute temperature of 300° K.

Hint: The most probable velocity is given by $v = \sqrt{\left(\frac{2kT}{m}\right)}$

Hence the momentum of the neutron is $mv = \sqrt{(2mkT)}$

Problem 11. At what velocity is the de Broglie wave-length of an alpha particle equal to that of a one kev X-ray.

[Hint: energy of the X-ray,

$$E=1 \text{ kev} = 10^3 \times 1.6 \times 10^{-12} \text{ ergs} = \frac{hc}{\lambda}$$

: Wave-length of x-ray,
$$\lambda = \frac{hc}{1.6 \times 10^{-9}}$$

This is also the wave-length of the α -particles and hence it is equal to $\frac{\lambda}{M_{-}v}$. Therefore,

$$\frac{hc}{1.6\times10^{-9}} = \frac{h}{M_{\alpha}v} \Rightarrow v = \frac{1.6\times10^{-9}}{cM_{\alpha}} \right].$$

Problem 12. Assuming the nuclear force between two protons to have a range $\approx 10^{-18}$ cm. due to π -meson exchange, use the uncertainty relation $\triangle E. \triangle t \approx h$ to calculate the approximate mass of the π -meson in Mev.

Sol. Since the range of the nuclear forces is 10^{-13} cm., the uncertainty in the time of the exchange of a meason is given by,

$$\triangle t = \frac{\triangle x}{c} = \frac{10^{-12}}{3 \times 10^{10}} = \frac{7}{3} \times 10^{-23} \text{ sec.}$$

From the uncertainty relation $\triangle E \triangle t \approx h$, we have the energy of the meson of the order of,

$$\Delta E \approx \frac{h}{\Delta t} = \frac{3 \times 6.62 \times 10^{-27}}{10^{-23}} = 19.86 \times 10^{-4} \text{ ergs.}$$

This energy is equal to a mass of,

$$m = \frac{19.86 \times 10^{-4}}{1.6 \times 10^{-12}} eV = 12.4 \times 10^{8} eV = 12.4 \times 10^{2} MeV \text{ (approx.)}$$

Problem 13. Excited nuclear states may have life time as short as 10^{-15} sec. How sharp would be these levels, (i. e. can we estimate the natural line width of the states).

Sol. Here $\Delta t = 10^{-15}$ sec. Therefore,

$$\triangle E \approx \frac{h}{\triangle t} = \frac{6.62 \times 10^{-27}}{10^{-15}} \approx 6.62 \times 10^{-12} \text{ ergs.}$$

Since $\triangle E = h \triangle v$, we get

$$\triangle v = \frac{\triangle E}{h} \approx \frac{1}{\triangle t} \approx \frac{1}{10^{-15}} \approx 10^{15} \text{ sec}^{-1},$$

this is the line width of the state.

Problem 14. Using uncertainty principle, calculate the size and energy of the ground state of hydrogen atom.

Sol. If $\triangle x$ and $\triangle p$ are uncertainties in the position and momentum of the electron in the ground state of hydrogen atom, then we have,

$$\triangle x. \triangle p \sim \hbar$$
$$\triangle p \approx \frac{\hbar}{\triangle x}$$

or.

The uncertainty in the kinetic energy of the electron may be written as,

$$\triangle T = \frac{1}{2} mv^2 = \frac{(\triangle p)^2}{2m} \approx \frac{\hbar^2}{2m(\triangle x)^2} \qquad ...(ii)$$

The uncertainty in the potential energy of the electron is,

$$\triangle V = -\frac{e^2}{\triangle x}...(iii)$$

So, the uncertainty in the total energy is given by

$$\triangle E = \triangle T + \triangle V \approx \frac{\hbar^2}{2m(\triangle x)^2} - \frac{e^2}{(\triangle x)} \qquad \dots (iv)$$

The ground state of the atom will correspond to a minimum value of $\triangle E$, therefore, $\frac{d(\triangle E)}{d(\triangle x)}$ must be equal to zero, i.e.,

$$\frac{d(\triangle E)}{d(\triangle x)} = \frac{-\hbar^2}{m(\triangle x)^3} + \frac{e^2}{(\triangle x)^2} = 0$$

$$\therefore \quad \triangle x \approx \frac{\hbar^2}{me^2} = \frac{(1.05 \times 10^{-27})^2}{9.1 \times 10^{-28} \times (4.8 \times 10^{-10})^2} \approx 0.5 \times 10^{-8} \text{ cm.}$$
...(v)

Putting this value of
$$\triangle x$$
 into (iv) we get,

$$\triangle E \approx \frac{\hbar^2}{2m} \cdot \frac{m^2 e^4}{\hbar^4} - e^2 \cdot \frac{me^2}{\hbar^2} = -\frac{me^4}{2\hbar^2}$$

$$= -13.6 \text{ eV}. \qquad ...(vi)$$

Thus, the radius of the first Bohr's orbit, which is of the order of the uncertainty in the position of the electron, is $a_0 \approx \triangle x \sim 0.5 \times 10^{-8}$ cm., and the corresponding energy is of the order of -13.6 eV.

Problem 15. Calculate the ground state energy of Helium atom using uncertainty principle.

Sol. Suppose, the two electrons of the Helium atom can be localized in the regions of dimensions $\triangle x_1$ and $\triangle x_2$ of the space. Then the spread in momenta (which is of the order of the momenta themselves) of the electrons would be given by,

$$\triangle p_1 \approx \frac{\hbar}{\triangle x_1}$$
 and $\triangle p_2 \approx \frac{\hbar}{\triangle x_2}$...(i)

Thus, the spread of the kinetic energy is given by-

$$\triangle E \approx \frac{\hbar^2}{2m} \left(\frac{1}{(\triangle x_1)^2} + \frac{1}{(\triangle x_2)^2} \right) \qquad \dots (ii)$$

The spread of the potential energy of interaction of the electrons with the nucleus of charge 2e is given by—

$$\triangle V_1 \simeq -2e^2 \left(\frac{1}{\triangle x_1} + \frac{1}{\triangle x_2} \right),$$
 ...(iii)

and the spread of the interaction energy between the electrons is,

$$\triangle V_2 \approx \frac{e^2}{\triangle x_1 + \triangle x_2}$$
 ...(iv)

$$\therefore \text{ Total energy, } \triangle E \approx \frac{\hbar^2}{2m} \left(\frac{1}{(\triangle x_1)^2} + \frac{1}{(\triangle x_2)^2} - 2e^2 \left(\frac{1}{\triangle x_1} + \frac{1}{\triangle x_2} \right) + \frac{e^2}{\triangle x_1 + \triangle x_2} \dots (v) \right)$$

For ground state, $\triangle E$ should be minimum. For it,

$$0 = \frac{d(\Delta E)}{d(\Delta x_1)} = \frac{-\hbar^2}{m(\Delta x_1)^3} + \frac{2e^2}{(\Delta x_1)^2} - \frac{e^2}{(\Delta x_1 + \Delta x_2)^2} \qquad \dots (vi)$$

and
$$0 = \frac{d(\Delta E)}{d(\Delta x_2)} = \frac{-\hbar^2}{m(\Delta x_2)^3} + \frac{2e^2}{m(\Delta x_2)^2} - \frac{e^2}{(\Delta x_1 + \Delta x_2)^2} \dots \text{(vii)}$$

Solving (vi) and (vii) we get-

$$\Delta x_1 = \Delta x_2 = \frac{4\hbar^2}{7me^2} \qquad ...(viii)$$

$$\therefore \Delta E \approx -\frac{49me^4}{16\hbar^2} \cong -83.3 \text{ eV}.$$

Problem 16. Use the uncertainty principle to estimate the ground state energy of a linear harmonic oscillator.

[Hint. If $\triangle p$ and $\triangle x$ are the spreads in the momentum and the position of the oscillator, its energy will be given by, $(\triangle p)^2 + 1 + 2 \cdot (\triangle p)^2$. Now for

 $E = \frac{(\triangle p)^2}{2m} + \frac{1}{2} m\omega^2 (\triangle x)^2. \text{ Now, from } \triangle x. \triangle p \approx \hbar, \text{ we have}$ $\triangle p \approx \frac{\hbar}{\triangle x}. \text{ Therefore,}$

$$E \approx \frac{\hbar^2}{m(\triangle x)^2} + \frac{1}{2} m\omega^2 (\triangle x)^2$$
.

This can be minimised to obtain the ground state energy of the oscillator.]

Problem 17. A neutron is confined to a nucleus of radius 5×10^{-13} cm. Calculate the minimum uncertainty in the momentum of the neutron and hence estimate the kinetic energy of the neutron inside the nucleus. What would be the kinetic energy for an electron if it had to be confined within a similar nucleus? Discuss the implications of the results obtained?

Sol. Radius of the nucleus= 5×10^{-13} cm. Hence the maximum uncertainty in the position of the neutron in the

nucleus may be equal to the diameter of the nucleus, i.e. $(\triangle x)_{max} \approx 2 \times 5 \times 10^{-13}$ cm = 10^{-12} cm.

According to uncertainty relation, $\triangle x \cdot \triangle p \approx \hbar$, if $\triangle x$ is maximum, $\triangle p$ must be minimum.

$$(\Delta p)_{min} \sim \frac{\hbar}{(\Delta x)_{max}} = \frac{1.05 \times 10^{-27}}{10^{-12}}$$

$$= 1.05 \times 10^{-15} \text{ gm. cm/sec.} ...(i)$$

Therefore, the kinetic energy of the neutron will be given by

$$E = \frac{(\triangle p)^2_{min}}{2M_n} \sim \frac{(1.05 \times 10^{-15})^2}{2 \times 1.67 \times 10^{-24}}; \text{ergs}$$

$$\approx 20.6 \text{ MeV}. \qquad ...(ii)$$

If we have an electron instead of the neutron, the kinetic energy will be given by

$$E_{electron} = \frac{(\Delta p)^2_{min}}{2m_e} \approx \frac{(1.05 \times 10^{-15})^2}{2 \times 9.1 \times 10^{-28}} \text{ ergs.}$$

$$\approx 346.7 \text{ MeV.} \qquad ...(iii)$$

From the result (ii), the average of the potential energy $\langle V \rangle$ of the nucleus must be negative and greater than the kinetic energy, therefore,

$$-\langle V \rangle \geqslant 20.6 MeV$$
, ...(iv)

this gives the order of the strength of the nuclear interaction

From (iii) we see that if the electrons exists in the nucleus their energy must be of the order of $346.7 \, MeV$. But in the β -decay, the electrons with energies exceeding a few MeV seldom emerge. Thus the free electrons cann't exist inside a nucleus and they are, in fact, created by the decay of a neutron into a proton at the instant the decay occurs.

Problem 18 Show that if a component of angular momentum of the electron in a hydrogen atom is known to be 2h within 5°, error, its angular orbital position in the plane perpendicular to that component cannot be specified at all

Sol. The uncertainty in the angular momentum is given to be,

$$\Delta J = \frac{5}{100} \times 2\hbar = \frac{\hbar}{10} \qquad \dots (i)$$

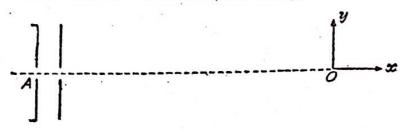
Therefore, from the uncertainty relation $\triangle J. \triangle \theta \approx \hbar$, we have the uncertainty in the measurement of the angle as

$$\Delta \theta = \frac{\hbar}{\Delta J} = \frac{\hbar}{\hbar/10} = 10 \text{ radians.} > 2\pi \text{ radians.}$$

Since the angle in a plane perpendicular to the component of angular momentum cannot be greater than 2π , the orbital angular position of the electron in the plane perpendicular to the given component of angular momentum cannot be specified at all.

Problem 19. A beam of silver atoms for a Stern-Gerlach experiment is produced by collimating atoms that vaporize from a silver held in a furnace at 1200°C. If the beam travel 1 metre, find the magnitude of the smallest spot that can be obtained at the detector.

Sol. It is given that the silver atoms are produced at a temperature of 1200°C. Therefore, the energy of these will be



given by, $E = \frac{3}{2}kT = \frac{1}{2}M_{Ag}.v_{x}^{2}$

$$v_x = \sqrt{\left(\frac{3kT}{M_{Ag}}\right)} = \left[\frac{3 \times 1.38 \times 10^{-10} \times (1200 + 273)}{108 \times 1.66 \times 10^{-24}}\right]^{1/2} \text{ cm/sec.}$$

$$= 5.832 \times 10^4 \text{ cm/sec.} \qquad \dots (i)$$

Time taken by the beam to reach the detector at O is given by

$$t = \frac{100}{v_x} \sec.$$

$$\therefore \quad (\triangle t)_{max} = \frac{100}{v_x} \sec. \qquad \dots (ii)$$

From the uncertainty relation, $(\triangle E)_{min}$. $(\triangle t)_{max} \approx \hbar$, we have

$$(\triangle E)_{min} \approx \frac{\hbar}{(\triangle t)_{max}} = \frac{\hbar v_x}{100} \text{ ergs}$$

$$\frac{(\triangle p)^2_{min}}{2M_{Ag}} = \frac{\hbar v_x}{100}$$

$$\therefore (\triangle p)_{min} \approx = \sqrt{\left(\frac{(2M_{Ag} \hbar v_x)}{100}\right)} \qquad \dots \text{(iii)}$$

or

This gives the minimum uncertainty in the measurement of the momentum of the atoms at the detector. Hence the maximum order of the size of the spot at the detector will be

$$(\Delta y)_{max.} \approx \frac{\hbar}{(\Delta p)_{min}} = \sqrt{\left(\frac{100\hbar}{2M_{Ag.}v_x}\right)}$$

$$= \left[\frac{100 \times 1.05 \times 10^{-27}}{108 \times 1.66 \times 10^{-24} \times 5.832 \times 10^4} \right]^{1/2} \text{ cm.}$$

$$\approx 6.97 \times 10^{-6} \text{ cm.}$$

This gives the smallest spot.

Problem 20. A ball of 0.1 gm is thrown with a velocity 103 em/sec through a circular hole of radius 10-4 cm. What is the uncertainty introduced in the angle of emergence?

Sol. We have
$$\triangle p \approx \frac{\hbar}{\triangle x} = \frac{1.05 \times 10^{-27}}{2 \times 10^{-4}} \approx 5 \times 10^{-24} \text{ gm cm/sec.}$$

$$p = mv = 0.1 \times 10^{3} = 10^{2} \text{ gm cm/sec.}$$

$$\therefore \theta \sim \frac{\triangle p}{p} = \frac{5 \times 10^{-24}}{10^{2}} \approx 5 \times 10^{-26} \text{ radians}$$

Problem 21. A particle is in a state given by the wave function $\psi(x, t) = e^{-\alpha x^2 - \beta t}$, where α and β are real constants.

- (i) Is it a stationary state?
- (ii) Show that the expectation values of p_x and x are zero.
- (iii) Does the result (ii) mean that the uncertainty relation $\triangle p_x \cdot \triangle x \geqslant 1$ is violated?

Explain your answer.

).

Sol. (i) The probability distribution for the given state of the particle is given by-

$$\psi^*\psi = e^{-2\alpha x^2 - 2\beta t} \tag{a}$$

Since this depends upon time, the given state is not a stationary

(ii) Expectation value of x is given by—
$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \, \psi \, dx = \int_{-\infty}^{+\infty} x e^{-2\alpha x^2 - 2\beta t} \, dx = 0$$

the integrand is an odd function of x) Expectation value of p_{\star} is given by

$$\langle p_x \rangle = -i \hbar \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$$= 2i \hbar \alpha \int_{-\infty}^{+\infty} x e^{-2\alpha x^2 - 2\beta t} = 0.$$

(iii) The result (ii) does not mean that Δp_x . $\Delta x \ge h$ is violated because Δp_x and Δx are defined by—

$$\triangle x = [\langle \{x - \langle x \rangle\}^2 \rangle]^{1/2}$$
 and $(\triangle p_x) = [\langle \{p_x - \langle p_x \rangle\}^2 \rangle]^{1/2}$
From the result (ii) we have—

$$\triangle x = [\langle x^2 \rangle]^{1/2}$$
 and $(\triangle p_x) = [\langle p_x^2 \rangle]^{1/2}$

The expectation values of x^2 and p_x^2 are not zero, and hence $\triangle p_x . \triangle x \geqslant h$ is not violated.

Problem 22. Show that for a three dimensional wave packet

$$\frac{d\langle x^2\rangle}{dt} = \frac{I}{m} \left[\langle xp_x\rangle + \langle p_x x\rangle \right]$$

Sol.
$$\langle x^2 \rangle = \int \psi^* x^2 \psi d^3 r$$

$$\therefore \frac{d\langle x^2\rangle}{dt} = \iint \left[\frac{\partial \psi^*}{\partial t} x^2 \psi + \psi^* x^2 \frac{\partial \psi}{\partial t} \right] d^3r$$

Substituting the values of $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \psi^*}{\partial t}$ from the Schroedinger equation and its complex conjugate, we can write

$$\frac{d\langle x^3\rangle}{dt} = \frac{i\hbar}{2m} \int [\psi^* \ x^2 \ \nabla^2 \psi - (\nabla^2 \psi^*) \ x^2 \ \psi] \ d^3r \qquad \dots(i)$$

Now,
$$\int (\nabla^2 \psi^*) \ x^2 \ \psi \ d^3r = \int \nabla . (x^2 \ \psi \ \nabla \psi^*) \ d^3r$$
$$-\int (\nabla \psi^*) . \nabla \ (x^2 \psi) \ d^3r.$$

The first integral on the right hand side can be transformed into a surface integral by using the Gauss's theorem. This will vanish for the surface at infinity, because ψ vanishes at infinity.

Once again, the first integral on the RHS can be transformed to a surface integral which would vanish. Thus,

$$\int (\nabla^2 \psi^*) \ x^2 \psi \ d^3r = \int \psi^* \ \nabla^2 (x^2 \psi) \ d^3r. \qquad \dots (ii)$$
Now
$$\nabla^2 (x^2 \psi) = \nabla \cdot \nabla (x^2 \psi) = \nabla \cdot [(\nabla x^2) \psi + x^2 (\nabla \psi)]$$

$$= (\nabla^2 x^2) \psi + (\nabla x^2) \cdot (\nabla \psi)$$

$$+ (\nabla x^2) \cdot (\nabla \psi) + x^2 (\nabla^2 \psi)$$

$$= 2\psi + 2x (\nabla \psi) + 2x (\nabla \psi) + x^2 (\nabla^2 \psi)$$

$$= 2\nabla (x\psi) + 2x (\nabla \psi) + x^2 (\nabla^2 \psi)$$

Substituting this value into (i) we obtain

$$\frac{d\langle \dot{x}^2 \rangle}{dt} = \frac{-i\hbar}{2m} \left[2 \int \psi^* \nabla x \psi \ d^3r + 2 \int \psi^* x \nabla \psi \ d^3r \right]$$

$$= \frac{1}{m} \left[\int \psi^* \left(-i\hbar \nabla \right) x \psi \ d^3r \right]$$

$$+ \int \psi^* x \left(-i\hbar \nabla \right) \psi \ d^3r \right]$$

$$= \frac{1}{m} \left[\langle p_x x \rangle + (x p_x) \right] = \frac{1}{m} \left[\langle x p_x \rangle + \langle p_x x \rangle \right]$$

Problem 23. Show that for a Gaussian wave-packet the uncertainty product is minimum.

Sol. According to the exact statement of the uncertatinty principle, the minimum uncertainty product is given by

$$\triangle x$$
. $\triangle p = \frac{\hbar}{2}$...(i)

The sign of equality in (i) occurs only if the sign of equality holds in the Schwarz inequality. For it the functions entering the Schwarz inequality should be proportional, i.e.

$$-i\hbar \frac{d\Psi}{dx} = C x \Psi \qquad ...(ii)$$

where C is a suitable multiplier. Integrating (ii) we get

$$\Psi = Ne^{-Cx^2/2i \, \hbar} \qquad \dots (iii)$$

Now, the relation of eqn. (129) should also have the equality sign for relation (i) to be true. For this,

$$\int i\hbar \frac{d\psi^*}{dx} x \psi d^3r = C^* \int x \psi^* x \psi d^3r \qquad \dots \text{(iv)}$$

should be purely imaginary. Hence C must be a purely imaginary number. For convenience, we write $C=i\hbar/C'$. Therefore,

$$\Psi = Ne^{-x^2/2C'} \qquad \dots (v)$$

For Ψ to vanish at infinity, C' must be positive. We write $C' = \sigma^2$, where σ is a real quantity. So

$$\Psi = Ne^{-x^2/2\sigma^2} \qquad \dots \text{(vi)}$$

This is a Gaussian curve. Thus the minimum wavepacket has the Gaussian shape. Gaussian wave-packet represents a

particle whose position and momentum can be determined simultaneously, as closely as the uncertainty principle permits.

. If we do not make the assumption $\langle x \rangle = \langle p \rangle = 0$ and proceed exactly as above, we shall obtain the result

we shall obtain the result

$$\Psi = N \exp \left[-\frac{(x - \langle x \rangle)^2}{2\sigma^2} \right] \exp \left[i \langle p \rangle x / \hbar \right] ... \text{(vii)}$$

This represents a wave-packet moving with average momentum $\langle p \rangle$. The quantity σ measures the width of the packet. constant N is determined by normalization, as follows

$$\int_{-\infty}^{+\infty} \psi^* \psi \ dx = |N|^2 \int_{-\infty}^{+\infty} e^{-(x-\langle x \rangle)^2/\sigma^2} \ dx = \sqrt{(\pi)} \ \sigma |N|^2 = 1$$

Hence,

$$\Psi(x, 0) = \frac{1}{\sqrt{[\sigma \sqrt{(\pi)}]}} \exp \left[\frac{-(x - \langle x \rangle)^2}{2\sigma^2} \right] \exp \left(i \frac{\langle p \rangle x}{\hbar} \right)$$
...(viii)

Generalized to three dimensions, the Gaussian packet can be written as

ten as
$$\Psi(\mathbf{r}, 0) = \frac{1}{[\sigma\sqrt{(\pi)}]^{8/2}} \exp \left[-\frac{|\mathbf{r}-\langle\mathbf{r}\rangle|^2}{2\sigma^2}\right] \exp \left[i\frac{\langle\mathbf{p}\rangle \cdot \mathbf{r}}{\hbar}\right] \dots (ix)$$

Problem 24. Show that a Gaussian wave-packet, spreads with

Suppose a wave-packet representing an electron has a dimension time. 10-8 cm. How long will it take for the wave-packet to spread to twice its dimension?

Sol. It has been seen in the previous problem that a Gaussian wave-packet at the initial time t=0 is given by;

wave-packet at the initial time.

$$\Psi(x, 0) = \frac{1}{\sqrt{[\sigma \sqrt{(\pi)}]}} \exp\left[\frac{-(x-\langle x \rangle)^2}{2\sigma^2}\right] \exp\left(i\frac{\langle p \rangle}{\hbar}x\right)...(i)$$

and this describes a particle for which the uncertainty relation has its minimum value, $\triangle x . \triangle p = \hbar/2$.

Now we shall consider the change of this wave-packet with time which will show that the packet spreads out with time. For it we know that a particle of momentum p and energy $E = \frac{p^2}{2m}$ can be represented by wave-packet:

$$\Psi(x,t) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} A(p) \exp\left[\frac{i}{\hbar} (px - Et) dp\right] ...(ii)$$

where the amplitude A(p) is given by the Fourier transform:

$$A(p) = \frac{1}{\sqrt{[(2\pi\hbar)]}} \int_{-\infty}^{+\infty} \Psi(x, t) \frac{-i}{e^{-\hbar}} (px - Et) dx \qquad \dots (iii)$$

Putting t=0 in (iii) and then using (i) into it we get

$$A(p) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{[\sigma\sqrt{(\pi)}]}} \exp\left[\frac{-(x-\langle x\rangle)^2}{2\sigma^2}\right] \exp\left[\frac{-i}{\hbar}(p-\langle p\rangle)x\right] dx.$$

Completing the square in($x-\langle x\rangle$), we get

$$A(p) = -\frac{1}{\sqrt{[2\pi \hbar \sigma \sqrt{(\pi)}]}} \int_{-\infty}^{+\infty} \exp\left[-\left\{\frac{x - \langle x \rangle}{\sqrt{(2)}\sigma} + \frac{\sigma i}{\sqrt{(2)}\hbar}(p - \langle p \rangle)\right\}^{2} - \frac{\sigma^{2}}{2\hbar^{2}}(p - \langle p \rangle)^{2} - \frac{i}{\hbar}(p - \langle p \rangle)\langle x \rangle\right] dx$$

Using $\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{(\pi)}$, we can evaluate the above integral.

We get-

$$A(p) = \frac{1}{\sqrt{[2\pi \hbar \sigma \sqrt{(\pi)}]}} \cdot \sqrt{(2)} \sqrt[4]{(\sigma)} \sqrt{(\pi)}.$$

$$\exp \left[\frac{-\sigma^2}{2 \hbar^2} (p - \langle p \rangle)^2 - \frac{i}{\hbar} (p - \langle p \rangle) \langle x \rangle \right]$$

$$= \sqrt{\left(\frac{\sigma}{\hbar \sqrt{(\pi)}} \right)} \exp \left[\frac{-\sigma^2}{2\hbar^2} (p - \langle p \rangle)^2 - \frac{i}{\hbar} (p - \langle p \rangle) \langle x \rangle \right] ...(iv)$$

The wavefunction in momentum space is therefore also a Gaussian function, but it is independent of time. Substituting (iv) into (ii) we get

$$\Psi(x, t) = \frac{1}{\sqrt{(2\pi \hbar)}} \cdot \sqrt{\left(\frac{\sigma}{\hbar \sqrt{(\pi)}}\right)} \int_{-\infty}^{+\infty} \exp\left[\frac{-\sigma^2}{2\hbar^2} (p - \langle p \rangle)^2\right]$$
$$\frac{-i}{\hbar} (p - \langle p \rangle) \langle x \rangle \exp\left[\frac{i}{\hbar} \left(px - \frac{p^2}{2m} t\right)\right] dp.$$

The integral appearing here is of the same form as that encountered in Eqn. (iii). We arrive at

$$\Psi(x, t) = \frac{\sigma}{\sqrt{[\sigma\sqrt{(\pi)} \alpha]}} \exp \left[\frac{-\sigma^2}{2 |\alpha|^4} \left\{x - \langle x \rangle - \frac{\langle p \rangle}{m} t\right\}^2\right]$$

$$\times \exp \left[\frac{1}{2 |\overline{\alpha}|^4} \left[\frac{2i}{\hbar} \sigma^4 \langle p \rangle \left(x - \frac{\langle p \rangle t}{2m}\right) - \frac{i\hbar t}{m} \left\{(x - \langle x \rangle)^2 - \frac{2t}{m} \langle p \rangle \langle x \rangle\right\}\right]$$
where $\alpha^2 = \sigma^2 + i\hbar t/m$(v)

It is evident that the centre of the wave-packet moves with speed $\langle p \rangle / m$. The probability density is obtained as:

$$|\Psi(x,t)|^2 = \frac{\sigma}{\sqrt{(\pi)|\alpha|^2}} \exp\left[-\frac{\sigma^2}{|\alpha|^4} \left\{x - \langle x \rangle - \frac{\langle p \rangle}{m} t\right\}^2\right]$$
...(vi)

When $|\psi|^2$ has the form e^{-x^2/σ^2} , then the width of the packet is given by $\sigma/\sqrt{2}$. Hence, the width of the wave-packet (v) is given by

$$\triangle x = \frac{\sqrt{\sigma}}{\sqrt{(2)}} \sqrt{\left(1 + \frac{\hbar^2 t^2}{m^2 \sigma^4}\right)} \qquad .. \text{ (vii)}$$

Clearly, the width of the packet increases with time.

Writing T^2 for $m^2 o^4/\hbar^2$, we can write

$$\triangle x = \frac{\sigma}{\sqrt{(2)}} \sqrt{\left\{1 + \left(\frac{t}{T}\right)^2\right\}} \qquad \dots \text{(viii)}$$

The packet will change its shape appreciably, only for $t>>T=\frac{m\sigma^2}{\hbar}$. Hence the time in which the width of the packet will become double is of the order of

$$t_0 \approx \frac{m\sigma^2}{\hbar} \approx \frac{m}{\hbar} (\triangle x)^2 \quad {::} \quad \triangle x \approx \sigma \text{ at } t = 0 \text{ from (vii)}}$$

In the present case $\triangle x \approx 10^{-8}$ cm. Therefore,

$$t_0 \approx \frac{m}{\hbar} 10^{-16} \approx \frac{9 \cdot 1 \times 10^{-28} \times 10^{-16}}{1 \cdot 05 \times 10^{-27}} \approx 10^{-16} \text{ secs.}$$

Problem 25. Calculate the probability current density corresponding to the wave function

$$\psi = \frac{e^{ik\tau}}{r} \qquad \dots (i)$$

where $r^2 = x^2 + y^2 + z^2$. Interpret the result physically.

Sol. The probability current density is given by

$$S = \frac{\hbar}{2im} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) = Re \cdot \left(\psi^* \frac{\hbar}{im} \nabla \psi \right) \qquad \dots (i)$$

We have $\psi = \frac{e^{ikr}}{r}$, $\psi^* = \frac{e^{-ikr}}{r}$

$$\therefore \qquad \nabla \psi = \left(\frac{ik}{r^2} e^{ikr} - \frac{1}{r^3} e^{ikr}\right) \hat{r},$$

and $\Delta \psi^* = \left(\frac{-ik}{r^2} e^{-ikr} - \frac{1}{r^3} e^{-ikr}\right) \hat{r}$ where \hat{r} is a unit vector along

r.

Therefore,
$$S = \frac{\hbar k}{m} \cdot \frac{\hat{r}}{r^2} = \frac{v}{r^2} \hat{r}$$
 ...(ii)

This represents the probability current for an isotropic stream of outgoing particles. The intensity falls off as $\frac{1}{r^2}$.

Problem 26. Show that for a normalized one-dimensional wave-packet,

$$\int_{-\infty}^{+\infty} S \, dx = \frac{\langle p_x \rangle}{m}.$$

Sol. We have S=Re. $\psi^*\left(\frac{-i\hbar}{m}\right)\frac{\partial \psi}{\partial x}$

$$\therefore \int_{-\infty}^{+\infty} S \, dx = \frac{1}{m} \operatorname{Re} \int_{-\infty}^{+\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi = \frac{1}{m} \operatorname{Re} \langle p_x \rangle = \frac{\langle p_x \rangle}{m}.$$

Problem 27. The normalized wave function of a particle on a straight line is given by

$$\psi(x) = \frac{1}{\sqrt{\{(\sigma) \sqrt{(\pi)}\}}} e^{-x^2/2\sigma^2} e^{ip_0x/\hbar} \qquad \dots (i)$$

- (a) Where is the particle most likely to be found?
- (b) What is the average momentum of the particle?

Sol. (a) The probability density for finding the particle is given by

$$|\psi(x)|^{2} = \frac{1}{\sigma\sqrt{(\pi)}} e^{-x^{2}/\sigma^{2}}$$
 ...(ii)

Clearly, it is maximum for x=0. Hence the particle is most likely to be found at x=0.

(b)
$$\langle p \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi^*(x) \frac{\partial \psi}{\partial x} dx$$

$$= -i\hbar \cdot \frac{1}{\sigma \sqrt{(\pi)}} \cdot \int_{-\infty}^{+\infty} e^{-x^2/\sigma^2} \left(\frac{ip_0}{\hbar} - \frac{2x}{2\sigma^2} \right) dx$$

$$= \frac{p_0}{\sigma \sqrt{(\pi)}} \int_{-\infty}^{+\infty} e^{-x^2/\sigma^2} dx + \frac{i\hbar}{\sqrt{(\pi)}\sigma^3} \int_{-\infty}^{+\infty} e^{-x^2/\sigma^2} x dx. \dots (iii)$$

The second integral vanishes, because the integrand is an odd function of x. The first integral can be evaluated from $\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{(\pi)}, \text{ we get}$

$$\langle p \rangle = \frac{p_0}{\sigma_{\sqrt{(\pi)}}} . \sigma \sqrt{(\pi)} = p_0.$$
 ...(iv)

Problem 28. The state of an oscillator of angular frequency ω is represented by

$$\psi(x) = e^{-m\omega x^2/\hbar} \qquad \dots (i)$$

- (a) What are the expectation values of the momentum and the position.
- (b) find the probability that the magnitude of the momentum is larger than $(m \hbar \omega)^{1/2}$.

Sol. (a) We have

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* \ x \ \psi \ dx = \int_{-\infty}^{\infty} e^{-2m\omega \ x^2/\hbar} \ x \ dx = 0.$$

$$\langle p \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx = i\hbar \int_{-\infty}^{+\infty} \frac{2x \, m \, \omega}{\hbar} e^{-2m\omega x^2/\hbar} = 0 \quad ... \text{(ii)}$$

(b) Find the Fourier transform a(p) of $\psi(x)$ by:

$$a(p) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} \psi(x) e^{-i/\hbar \cdot px} dx. ...(iii)$$

Then $|a(p)|^2$ is the momentum probability density. Hence the probability that the momentum is large, then $(m\hbar\omega)^{1/2}$ is given by

$$\int_{(m\hbar\omega)^{1/2}}^{\infty} |a(p)|^2 dp \qquad ...(iv)$$

2.1. WHAT IS AN OPERATOR:

According to the physical significance of wave function, the wavefunction belonging to any physical system contains all possible information about the system. But just by looking at the wavefunction of any system, we cannot tell anything about the system. In order to deduce the observable properties of the system, we have to perform mathematical operations upon the wavefunction of that system. Operators are the symbols for performing these operations, ie, the symbols which when written infront of a function will change it into another function of the same variables according to a definite law This can be represented as

$$A\psi = \psi'$$
. ...(1)

This means that the function ψ' is the result of applying the operation represented by operator A to the function ψ . For example, multiplication by the scalar x may be considered as an operator, as

$$x(x^3+1)=x^4+x$$
 ...(2)

In operator language, when the operator A=x, operates on the function $\psi=x^3+1$, it is changed into another function $\psi'=x^4+x$.

As another example, differentiation with respect to x, may also be considered as an operator, as

$$\frac{d}{dx}(x^3+1) = 3x^2 \dots (3)$$

i.e. when the operator $A = \frac{d}{dx}$, operates on the function $\psi = x^3 + 1$, it changes ψ to $\psi' = 3x^2$.

2.2. LINEAR OPERATOR:

An operator A is called a linear operator if it satisfies the following rules

$$A (\psi_1 + \psi_2) = A\psi_1 + A\psi_2$$
(4a)

and $A(c\psi_1)=cA\psi_1,$...(4b)

where ψ_1 and ψ_2 are given functions and c is a scalar constant. As is apparent, the examples cited above are linear. Two linear

operators of fundamental importance are the null or zero operator, defined by

 $O\psi=0,$...(5)

which destroys the function to which it is applied, and the unit or identity operator I,

which makes no change in the function on which it operates.

It should be noted that all the operators of quantum mechanical importance will be linear operators.

2.3. ALGEBRA OF LINEAR OPERATORS:

If the operators A and B are such that for every function ψ ,

 $A\psi = B\psi, \qquad \dots (7)$

then A and B are defined to be equal to each other, and we write it as A=B. The operators for which the above equation does not hold are termed as unequal operators.

: If the operators A, B and C are-of such nature that

 $C\psi = A\psi + B\psi, \qquad \dots (8)$

for every function ψ for which the operations involved in equation (8) can be carried out, then C is defined to be the sum of A and B and we write it as C = A + B

*Similarly, if

 $C\psi = A (B\psi), \qquad \dots (9)$

then C is the product of A and B. It should be noted that AB and BA may not be equal. For example

at
$$x\left(\frac{d\psi}{dx}\right) = x\frac{d\psi}{dx}.$$

$$\frac{d}{dx}(x\psi) = x\frac{d\psi}{dx} + \psi,$$

But

whence if $A = \frac{d}{dx}$ and B = x, then $AB \neq BA$. Thus the order of the

operators in the product is very important and cannot be changed in general

If for operators A and B in some particular case, AB=BA, then A and B are said to *commute* with each other. For commuting operators A and B,

$$AB-BA=0$$

or, in symbolic form

[A, B] = 0 ...(10)

where $[A, B] = (AB \quad BA)$ and is called the *commutator bracket* of A and B operators If for operators A and B, $[A, B] \neq 0$, then the operators A and B will be called as *non-commuting operators*.

The square of an operator A is defined as $A^2 = A \cdot A \qquad \dots (11)$

Similarly, $A^3 = A^2 \cdot A = A \cdot A^2$ and other higher powers can also be defined.

If two operators A and B are related by the equation AB = BA = I...(12)

then they are called the reciprocal of each other, and we write $A^{-1}=B \text{ and } B^{-1}=A \qquad ...(13)$

2.4. EIGEN-FUNCTION AND EIGEN-VALUE OF AN OPE-RATOR:

We have written the result of the operation of an operator A upon a wavefunction ψ as $A\psi = \psi'$ where ψ' is a function of the same variables as ψ . In general ψ' will be quite different from ψ' But in some cases ψ' may come out to be some constant multiple of the function ψ , i e., ...(14)

 $A\psi = \lambda \psi$, where λ is a constant In such cases ψ is called an eigenfunction of the operator A, λ is called the eigenvalue of A associated with the function ψ . Equation (14) is called the eigenvalue equation for the operator A.

As an example, if we take $\psi = \cos 4x$ and $\Lambda = \frac{d^2}{dx^3}$, then

$$\frac{d^2}{dx^2}\cos 4x = -16\cos 4x,$$
$$A\psi = -16\psi,$$

we say that the number -16 is an eigenvalue of the operator $\frac{d^2}{dx^2}$ associated with the function $\cos 4x$.

In order to understand the importance of operators in Quantum Mechanics, it shouled be noted that each dynamical variable of the motion of a system can be represented by a linear operator and the eigenvalues of that operator give the result of a precise measurement of the dynamical variable represented by that operator. In the succeeding chapters we will see that, $-i\hbar \nabla$ and $i\hbar \frac{\partial l}{\partial t}$, the operators correspoding to the linear momentum and the total energy of a system, respectively, give the momentum and the energy of the system when operated on their respective eigenfunctions,

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$$(-i\hbar \nabla) \psi = p\psi ; \psi = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p.r/\hbar}} ...(15)$$

and
$$\left(i\hbar \frac{\partial}{\partial t}\right)\psi = E\psi \; ; \; \psi = u \; (\mathbf{r}) \; e^{-iEt/\hbar} \qquad ...(16)$$

In the above equations p and E are the eigenvalues of the momentum and the energy operators; respectively, and give the momentum and the total energy of the system. We have also defined the Hamiltonian operator,

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}), \qquad \dots (17)$$

which gives the total energy of a time independent system. In the succeeding chapters we shall come across some more operators, which will correspond to the dynamical variables of a system, and shall study their properties. In the above examples, the momentum and the energy operators have continuous sets of eigen values. The set of eigenvalues and eigenfunctions may also be discrete. In general, for a bound state, the sets of eigenvalues and eigenfunctions are discrete sets, while for a free state, these are continuous sets.

Thus we see that if 'F' is the operator corresponding to some dynamical variable and if we make a measurement of that variable for a system represented by a statefunction ' ψ ', then the result of that measurement will be ' λ ' and is given by

$$F\psi = \lambda \psi$$
. ...(18)

Also, the average value of the dynamical variable represented by F in a series of measurements performed on an ensemble of systems in identical states ψ is given by

$$\langle F \rangle = \frac{\int \psi^* \ F \psi \ d^3 r}{\int \psi^* \ \psi \ d^3 r}. \tag{19}$$

Substituting (18) in (19), we get

$$\langle F \rangle = \frac{\int \psi^* \lambda \psi \ d^3 r}{\int \psi^* \psi \ d^3 r} = \lambda. \tag{20}$$

Thus the average value of an operator F in a state represented by an eigenfunction of F is the corresponding eigenvalue. Since the physical quantity corresponding to F is an observable, it must be real. Thus the eigenvalues of the operators corresponding to the dynamical variables are real numbers.

2.5. ORTHONORMAL SET OF EIGENFUNCTIONS:

Let the eigen values be discrete and the corresponding eigen-

functions be represented by $\psi_1, \psi_2, \psi_3, ..., \psi_m$, etc. If for any two eigenfunctions ψ_m and ψ_n , we have the condition

 $\int \psi_m^* \psi_n d^3r = 0$; $m \neq n$ and m, n = 1, 2, 3, ...etc. ...(21) where the integration is over the space in which the functions are defined, then the functions ψ_m and ψ_n are called as *orthogonal* to each other and the set of the eigenfunctions will be called as an orthogonal set of eigenfunctions.

The integral of the product of ψ_m^* and ψ_n in (21) can also be represented by the symbol $(\psi_m, \psi_n) = (\psi_n, \psi_m)^*$ and is known as the scalar product of the functions ψ_m and ψ_n . Thus

$$(\psi_m, \psi_n) \equiv (\psi_n, \psi_m)^* \equiv \int \psi_m^* \psi_n d^3r \qquad \dots (22)$$

If the relation

.

$$(\psi_m, \psi_n) \equiv (\psi_n, \psi_m)^* \equiv \int \psi_m^* \psi_n d^3r = 1 \text{ for } m = n = 1, 2, 3, \dots \text{etc.}$$

holds, then the set of the eigenfunctions will be called as normalized set of eigenfunctions.

If the set of the eigenfunctions is orthogonal as well as normalized, then we shall call it as an orthonormal set of eigenfunctions. In general, the orthonormal set of eigenfunctions satisfy the condition,

$$(\psi_m, \psi_n) \equiv (\psi_n, \psi_m)^* \equiv \int \psi_m^* \psi_n \, d^3r = \delta_{mn} \qquad \dots (24)$$
 where δ_{mn} is the Kronecker delta defined as

$$\delta_{mn} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n. \end{cases}$$

1-2-6. COMPLETE SET OF EIGENFUNCTIONS:

Let us consider a linear combination of the members of an orthonormal set of eigenfunctions of some operator,

$$\sum_{i=1}^{\infty} c_i \psi_i, \qquad \dots (25)$$

where c_t 's are complex numbers.

If the series (26) converges, it defines a function

$$f = \sum_{i=1}^{\infty} c_i \psi_i \qquad \dots (26)$$

A large number of functions can be expressed as a sum of the above type. The set of functions ψ_i is said to be a *complete set* with respect to the members of such a class of functions.

We assert that any arbitrary wavefunction '\psi' of physical interest can always be written as a linear combination of eigenstates of the

operators corresponding to the dynamical variables of a system which are observable and measurable experimentally; i.e.,

$$\psi = \sum_{l=1}^{\infty} c_l \psi_i, \qquad \dots (27)$$

where ψ_i 's are the eigenfunctions of an operator corresponding to the dynamical observable of the system. Thus the set of the functions ψ_i is complete w.r.t. all the wavefunctions ' ψ ' of physical interest. To find the coefficients c_i , we make use of the orthonormality of the eigenfunctions ψ_i . Multiplying (27) by ψ_i^* and integrating over, we get

$$\int \psi_{j}^{*} \psi \ d^{3}r = \sum_{i=1}^{\infty} c_{i} \int \psi_{i}^{*} \psi_{i} \ d^{3}r$$

$$= \sum_{i=1}^{\infty} c_{i} \delta_{ji} = c_{j}$$

$$\vdots c_{i} = \int \psi_{i}^{*} \psi \ d^{3}r \equiv (\psi_{i}, \psi) \qquad \dots (28)$$

In order to understand the physical significance of the expansion coefficients, let us suppose that $\{\psi_1, \psi_2, \dots\}$ is an orthonormal set of eigenfunctions of some operator A and $\{\lambda_1, \lambda_2, \dots\}$ is the set of the corresponding eigenvalues; *i.e.*

$$A \psi_{i} = \lambda_{i} \psi_{i}$$
; $i = 1, 2, ...$ etc. ...(29)

Now, if we make a measurement of dynamical variable A on the system in the state ψ , it will be given by the average value of A,

$$\langle A \rangle = (\psi, A\psi) = (\sum_{i} c_{i} \psi_{i}, A \sum_{j} c_{j} \psi_{j})$$

$$= (\sum_{i} c_{i} \psi_{i}, \sum_{j} c_{j} \lambda_{j} \psi_{j}) = \sum_{i} \lambda_{j} c_{i} * c_{j} (\psi_{i}, \psi_{j})$$

$$= \sum_{i} \lambda_{j} c_{i} * c_{j} \delta_{i,j} = \sum_{i} \lambda_{i} c_{i} * c_{i}$$
or
$$\langle A \rangle = \sum_{i} \lambda_{i} |c_{i}|^{2} \dots (30)$$

If $P(\lambda_i)$ denotes the probability that an individual measurement will give the value λ_i , then by definition

$$\langle A \rangle = \sum_{i} \lambda_{i} P(\lambda_{i}) \qquad \dots (31)$$

Comparing (30) and (31), we get $P(\lambda_l) = c_l l^2,$

i.e. the absolute square of the coefficient of expansion in the expansion of ψ in the eigenfunctions of A is the probability that a measurement of A will give the value λ_i .

If an operator has a continuous set of eigenvalues, then the summations in the above expressions will be replaced by integrations. As an example, we have seen that the momentum operator, $-i\hbar\nabla$, has a continuous set of eigenvalues 'p' with eigenfunctions,

$$\psi_{p} = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} \dots (32)$$

The Fourier transform.

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$$\psi(\mathbf{r},t) = \int \phi(\mathbf{p},t) \psi_{\mathbf{p}} d^{3} p, \qquad \dots (33)$$

is a representation of the state ψ (r, t) as a liner superposition of the states ψ_p ; i.e., it is analogous to the expansion (27). The formula (28) for the expansion coefficients becomes,

$$\phi(\mathbf{p}, t) = (\psi_p, \psi) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \psi(\mathbf{r}, t) d^3r \qquad ...(34)$$

To summarize, we have said that every physical quantity can be represented by an operator with eigenfunctions $\{\psi_1, \psi_2, ..., \psi_l, ...\}$, which forms a complete set of orthonormal functions w.r.t. every physical state ψ in the sense that every arbitrary physical state ψ can be written as a sum of the form (27) where the coefficients are defined by eqn. (28).

2.7. COMPLETENESS RELATION.

Let $\{\psi_1, \psi_2, ..., \psi_l, ...\}$ be a complete set of eigenfunctions of some operator corresponding to a dynamical observable of some physical system. Then an arbitrary state ψ can be written as,

$$\psi = \sum_{i=1}^{\infty} c_i \psi_i \; ; \; c_i = (\psi_i, \psi). \tag{35}$$

Now, we have :

$$(\psi, \psi) = \begin{pmatrix} \sum_{i=1}^{\infty} c_i \psi_i, \sum_{j=1}^{\infty} c_j \psi_j \end{pmatrix} = \sum_{i,j=1}^{\infty} c_i^* c_j (\psi_i, \psi_j)$$

$$= \sum_{i,j=1}^{\infty} c_i^* c_j \delta_{ij} = \sum_{i=1}^{\infty} c_i^* c_i = \sum_{i=1}^{\infty} |c_i|^2$$

$$(36)$$

Equation (36) is called the completeness relation for the given set, because, it is the necessary as well as sufficient condition for a set of functions to be complete. To prove this, we shall show that

 $\sum_{i=1}^{\infty} c_i \, \psi_i \text{ indeed converges to } \psi, \text{ if the relation (36) is satisfied.}$

The quantity,
$$\epsilon_n = \int |\psi - \sum_{i=1}^n c_i \psi_i|^2 d^3r, \qquad \dots (37)$$

is a positive number which measures the departure of $\Sigma c_i \psi_i$ from ψ . If $\epsilon_n \to 0$ as $n \to \infty$, then there will be no departure of Σ c_i ψ_i

from ψ and we can say that $\sum_{i=1}^{\infty} c_i \psi_i$ converges to ψ . Such a convergence is called as the convergence in the mean. Now we have,

$$\lim_{n\to\infty} \lim_{\epsilon_n = \infty} \lim_{n\to\infty} |\psi - \sum_{i=1}^n c_i \psi_i|^2 d^3r$$

$$= \lim_{n\to\infty} \int \left(\psi^* - \sum_{i=1}^n c_i^* \psi_i^* \right) \left(\psi - \sum_{j=1}^n c_j \psi_j \right) d^3r$$

$$= \int \psi^* \psi \ d^3r - \lim_{n \to \infty} \sum_{i=1}^n c_i^* \int \psi_i^* \psi \ d^3r - \lim_{n \to \infty} \sum_{j=1}^n c_j \int \psi^* \psi_j \ d^3r$$

$$+\lim_{n\to\infty}\sum_{i,j=1}^n\int c_i^*\psi_i^*c_j\psi_j\,d^3r$$

$$=\int \psi^* \psi \, d^3r - \lim_{n\to\infty} \sum_{i=1}^n c_i^* c_i - \lim_{n\to\infty} \sum_{j=1}^n c_j c_j^*$$

$$+\lim_{n\to\infty}\sum_{i=1}^{n}c_{i}*c_{i}\delta_{i},$$

 $+\lim_{n\to\infty}\sum_{i,j=1}^{n}c_{i}*c_{i}\delta_{i,j}$ {: $\int \psi_{i}*\psi_{i}d^{3}r=c_{i}*$ and $\int \psi_{i}*\psi_{i}d^{3}r=\delta_{i,j}$ }

$$= \int \psi^* \psi \, d^3r - \lim_{n \to \infty} \sum_{i=1}^n |c_i|^2 - \lim_{n \to \infty} \sum_{j=1}^n c_j c_j^* + \lim_{n \to \infty} \sum_{j=1}^n c_j^* c_j$$

(On carrying out the sum over i in the last term on the right hand side)

$$= \int \psi^* \psi \ d^3r - \sum_{i=1}^{\infty} |c_i|^2 \qquad ...(38)$$

=0 (if equation (36) hold good)

Conversely, if $\psi = \sum_{c_i \psi_i} c_i \psi_i$, then $\lim_{n \to \infty} \epsilon_n = 0$ in the equation (37). Or from (38) we have,

$$\int \psi^* \psi \ d^3r - \sum_{\ell=1}^{\infty} |c_{\ell}|^2 = 0$$

$$\int \psi^* \psi \ d^3r \equiv (\psi, \psi) = \sum_{\ell=1}^{\infty} |c_{\ell}|^2.$$

This proves that the completeness relation is the necessary as well as the sufficient condition for a set to be complete.

HERMITIAN OPERATOR'S:

An operator A, representing some observable, must for state ψ , yield an expectation value.

$$\langle A \rangle = \int \psi^* A \psi \ d^3r = (\psi, A \psi),$$
 (39)

which is a real number. Consequently, A must satisfy the condition,

or
$$\int (\int \psi^* A\psi d^3r)^* = \int \psi^* A\psi d^3r$$
or
$$\int (A\psi)^* \psi d^3r = \int \psi^* A\psi d^3r$$
or equivalently,
$$(A\psi, \psi) = (\psi, A\psi)$$
...(40)

A linear operator which obeys the rule (40. is called a Hermitian Operator. More generally, a Hermitian operator satisfies the relation.

$$(\psi, A\phi) = (A\psi, \phi) \qquad \dots (41)$$

for any two functions ψ and ϕ . To prove this for a Hermitian operator Λ , we have for the state-function $(\psi + \phi)$,

$$\int (\psi + \phi)^* A(\psi + \phi) d^3r = \int [A(\psi + \phi)]^* (\psi + \phi) d^3r$$

{: A is Hermitian}

or
$$\int \psi^* A\psi d^3r + \int \psi^* A\phi d^3r + \int \phi^* A\psi d^3r + \int \phi^* A\phi d^3r$$

= $\int (A\psi)^* \psi d^3r + \int (A\phi)^* \psi d^3r + \int (A\psi)^* \phi d^3r + \int (A\phi)^* \phi d^3r$

or
$$\int \psi^* A\phi \ d^3r + \int \phi^* A\psi \ d^3r = \int (A\phi)^* \psi \ d^3r + \int (A\psi)^* \phi \ d^3r \dots (42)$$
{ : A is Hermitian, therefore, $\int \psi^* A\psi \ d^3r = \int (A\psi)^* \psi \ d^3r$
and $\int \phi^* A\phi \ d^3r = \int (A\phi)^* \phi \ d^3r$ }

Again, for the state function $(\psi + i\phi)$, we have

$$\int (\psi + i\phi)^* A (\psi + i\phi) d^3r = \int [A (\psi + i\phi)]^* (\psi + i\phi) d^3e$$

Or
$$\int \psi^* A\psi d^3r + \int \phi^* A\phi d^3r + i \int \psi^* A\phi d^3r - i \int \phi^* A\psi d^3r$$

= $\int (A\psi)^* \psi d^3r + \int (A\phi)^* \phi d^3r + i \int (A\psi)^* \phi d^3r$

-i [(A4)* \ d3r

or
$$\int \psi^* A\phi d^3r - \int \phi^* A\psi d^3r = \int (A\psi)^* \psi d^3r - \int (A\phi)^* \psi d^3r \dots (43)$$

Now, both the eqns. (42) and (43) holds good simultaneously,

if
$$\int \psi^* A\phi \ d^3r = \int (A\psi)^* \phi \ d^3r$$
 i.e., $(\psi, A\phi) = (A\psi, \phi)$ and $\int \phi^* A\psi \ d^3r = \int (A\phi)^* \psi \ d^3r$ i.e., $(\phi, A\psi) = (A\phi, \psi)$.

This proves the assertion of eqn. (41), for a Hermitian operator, i.e., the operator can be applied to either factor in the scalar product.

2.9. PROPERTIES OF HERMITIAN OPERATORS:

Following are some important properties of the Hermitian operators.

(I) Sum of two Hermitian operators is Hermitian.

Proof. Let A and B be two Hermitian operators. Then, for any two arbitrary functions ψ and ϕ , we have

$$\int \psi^* A\phi \ d^3r = \int (A\psi)^* \phi \ d^3r$$
$$\int \psi^* B\phi \ d^3r = \int (B\psi)^* \phi \ d^3r$$

and

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Adding these equations, we get

$$\int \psi^* A\phi \ d^3r + \int \psi^* B\phi \ d^3r = \int (A\psi)^* \phi \ d^3r + \int (B\psi)^* \phi \ d^3r$$

$$\int \psi^* (A+B) \phi \ d^3r = \int [(A+B) \psi]^* \phi \ d^3r$$

This shows that (A+B) is a Hermitian operator.

(II) Product of commuting Hermitian operators is Hermitian.

Proof. Let A and B be two commuting (AB=BA) Hermitian operators.

and \$\psi\$ and \$\psi\$ be two arbitrary wave-functions.

Then, for Hermitian operator A and the states ψ and $B\phi$, we have $\int \psi^* A(B\phi) d^3r = \int (A\psi)^* B\phi d^3r \qquad \dots (44)$

Also for Hermitian operator B and the states $A\psi$ and ϕ , we have $\int (A\psi)^* B\phi \ d^3r = \int [B(A\psi)]^* \phi \ d^3r \qquad ...(45)$

This shows that AB is Hermitian.

(III) Every eigenvalue of a Hermitian Operator is real.

Proof. Let \$\psi\$ be any eigenfunction of a Hermitian operator \$A\$ with eigenvalue \$\lambda\$, then

$$\int \phi^* A \phi \ d^3r = \int (A \phi)^* \phi \ d^3r$$

$$\int \phi^* \lambda \psi \ d^3r = \int (\lambda \phi)^* \phi \ d^3r$$

$$\lambda \int \phi^* \psi \ d^3r = \lambda^* \int \phi^* \phi \ d^3r.$$
...(46)

Since $\psi \neq 0$, therefore, $\int \psi^* \psi \ d^3r \neq 0$. Hence eqn (46) gives,

$$\lambda = \lambda^*$$
 or λ is real.

(IV) Two eigenfunctions of a Hermitian operator belonging to different eigenvalues are orthogonal.

Proof. Let A be a Hermitian operator, and ψ_1 , ψ_2 be its two eigenfunctions with eigenvalues λ_1 and λ_2 which are different;

i.e.,
$$A\psi_1 = \lambda_1 \psi_1$$
; $A\psi_2 = \lambda_2 \psi_2$; $\lambda_1 \neq \lambda_2$.

Since A is Hermitian, therefore by definition

$$(\psi_1, A\psi_2) = (A\psi_1, \psi_2)$$
 or $(\psi_1, \lambda_2\psi_2) = (\lambda_1\psi_1, \psi_2)$

or
$$\lambda_2 (\psi_1, \psi_2) = \lambda_1^* (\psi_1, \psi_2)$$
 or $\lambda_2 (\psi_1, \psi_2) = \lambda_1 (\psi_1, \psi_2)$

(: eigenvalue λ_1 of a Hermitian operator must be real)

or
$$(\lambda_1 - \lambda_2) (\psi_1, \psi_2) = 0$$
$$\Rightarrow (\psi_1, \psi_2) = 0 \qquad \{ :: \lambda_1 \neq \lambda_2 \Rightarrow (\lambda_1 - \lambda_2) \neq 0 \}.$$

This shows that ψ_1 and ψ_2 are orthogonal to each other...

(V) If ψ_1 and ψ_2 are two linearly independent eigenfunctions of A, belonging to the same eigenvalue, then every linear combination of ψ_1 and ψ_2 will also be an eigenfunction with the same eigenvalue.

Proof. Let ψ_1 and ψ_2 both have the eigenvalue λ ,

i.e.,
$$A\psi_1 = \lambda \psi_1$$
 and $A\psi_2 = \lambda \psi_2$.

In this case, λ is said to be degenerate w r.t. ψ_1 and ψ_2 .

Now for any linear combination $c_1\psi_1+c_2\psi_2$ of ψ_1 and ψ_2 , we have

$$A (c_1\psi_1 + c_2\psi_2) = c_1A\psi_1 + c_2A\psi_2$$

= $\lambda (c_1\psi_1 + c_2\psi_2).$

Here C_1 and C_2 are arbitrary constants. It will be shown in the next chapter that by selecting these constants properly, we can always construct orthogonal eigen-functions.

2:10. ADJOINT OF AN OPERATOR:

Let A be an arbitrary operator, not necessarily Hermitian, then we define its adjoint A† (read as A-dagger) by the equation

$$\int \psi^* A^{\dagger} \phi d^3 r = \int (A\psi)^* \phi d^3 r$$
or equivalently $(\psi, A^{\dagger} \phi) = (A\psi, \phi),$
where ψ and ϕ are two arbitrary state-functions.

(47)

If A is Hermitian, then
$$(\psi, A\phi) = (A\psi, \phi), \qquad \dots (48)$$

Comparing (47) and (48), we get $A\dagger = A$; i.e., A is Hermitian, if it is self-adjoint. The converse of this is also true. Hence, Hermitian is a synonym for self-adjoint.

If A and B are two arbitrary operators, then the adjoint of their product is given by

$$(AB)\dagger = B\dagger A\dagger$$
; ...(49)

i.e., the order of the factors is reversed. To show it, we have from the definition

$$\int \psi^* (AB)^{\dagger} \phi \ d^3r = \int (AB\psi)^* \phi \ d^3r = \int (B\psi)^* A^{\dagger} \phi \ d^3r$$
$$= \int \psi^* B^{\dagger} A^{\dagger} \phi \ d^3r.$$

But ψ and ϕ are arbitrary, hence (49) follows. If A and B are both Hermitian,

$$(AB)\dagger = B\dagger A\dagger = BA.$$

From it we see that AB will be Hermitian if and only if BA=AB, i e., if and only if A and B commutes as we have proved in the last article.

2:11. SIMULTANEOUS MEASURABILITY AND COMMUTATORS:

If A and B are two linear operators corresponding to certain dynamical observables and ψ is a wave-function satisfying both the equations,

$$A\psi = \alpha \psi$$
 and $B\psi = \beta \psi$, ...(50)

then ψ is called a *simultaneous eigenfunction* of A and B; i.e., the value of the quantities corresponding to the operators A and B can be measured simultaneously for the system or particle represented by the wave-function ψ .

Now, we shall find the condition satisfied by the operators A and B for which a simultaneous eigenfunction exists. For it, we see from equation (50) that

$$BA\psi = B(\alpha\psi) = \alpha(B\psi) = \alpha\beta\psi$$

and

$$AB\psi = A (\beta\psi) = \beta (A\psi) = \beta \alpha \psi.$$

Subtracting the above two equations from one another,

we get
$$(AB-BA) \psi=0.$$
 ...(51)

From this equation we see that (AB - BA) = [A, B] = 0, i.e., A and B commutes. Hence, it is necessary for two operators to commute with each other for having a simultaneous eigenfunction. We can show that it is a sufficient condition also; i.e., the eigen-

functions of commuting operators can always be constructed in such a way that they are simultaneous eigenfunctions. To prove it, let A and B be two commuting operators;

i.e.,
$$[A, B] = AB - BA = 0$$
,

and let ψ be an eigenfunction of A with an eigenvalue α ,

$$A\psi = \alpha \psi$$
.

Now we have to find out an eigenfunction, which is a simultaneous eigenfunction of A and B both. For it we have,

$$AB\psi = BA\psi = B\alpha\psi = \alpha B\psi,$$

$$A(B\psi) = \alpha(B\psi).$$

If $B\psi \neq 0$, then we see from this equation that $(B\psi)$ is also an eigenfunction of A with the eigenvalue α . Now, two cases may be distinguished.

(I) α is non-degenerate. By non-degeneracy we mean that there is only one eigenfunction corresponding to every eigenvalue. Then, the function $(\beta\psi)$ must be a constant multiple of ψ ,

i.e.,
$$B\psi = \beta \psi$$
; β is a complex number.

This shows that ψ is also an eigenfunction of B with the eigenvalue β .

(II) α is degenerate. By degeneracy we mean that there are more than one eigenfunction corresponding to an eigenvalue. Let us suppose that α is an *n*-fold degenerate eigenvalue of A; i.e., there exists 'n' linearly independent* eigenfunctions $\{\psi_1, \psi_2, ..., \psi_n\}$ of A with the same eigenvalue α ,

$$A\psi_i = \alpha \psi_i$$
; $i=1, 2, ..., n$.

From this equation we have,

$$A(B\psi_i)=BA\psi_i=B\alpha\psi_i=\alpha(B\psi_i)$$
;

*By linear independence of the functions we mean that no function of the given set of functions can be expressed in terms of the other functions of the set. Mathematically, the set of functions $\{\psi_1, \psi_2, ..., \psi_n\}$ will be linearly independent, if and only if, the equation

$$c_1\psi_1 + c_2\psi_0 + \dots + c_n\psi_n = 0$$

$$\sum_{i=1}^n c_i\psi_i = 0,$$

or

i.e.

is satisfied for $c_1 = c_2 = ... c_n = 0$ and for no other values of c_1

Also see section 3.1 C.

i.e., $(B\psi_i)$ is also an eigenfunction of A with the same eigenvalue α . If $(B\psi_i)$ is linearly independent of ψ_i (i=1 to n), then we shall have a set of (n+1) linearly independent eigenfunctions, $\{\psi_1, \psi_2, \ldots, \psi_n, B\psi_i\}$, of A with the same eigenvalue α ; i.e., α will be an (n+1) fold degenerate eigenvalue, which violates the hypothesis that α is only an n-fold degenerate eigenvalue. So, $B\psi_i$ is not linearly independent of $\{\psi_1, \psi_2, \ldots, \psi_n\}$ and can be expressed in terms of them as:

$$B\psi_{l} = \sum_{k=1}^{n} c_{ik} \psi_{k}, \qquad \dots (52)$$

where cik's are the coefficients of expansion.

Now, from the above equation we cannot say that ψ_i 's are also the eigenfunctions of the operator B. However, we can construct a new set of eigenfunctions $\overline{\psi}_i$ of A with eigenvalue α , which are linear combinations of ψ_i 's, and which are at the same time eigenfunctions of B. We write

$$\overline{\psi}_{j} = \sum_{l=1}^{n} d_{jl} \ \psi_{l}$$

and demand that

$$B\overline{\psi}_{j} = \beta\overline{\psi}_{j} \text{ or } B \sum_{l=1}^{n} d_{jl} \psi_{l} = \beta \sum_{l=1}^{n} d_{jl} \psi_{l}$$
or
$$\sum_{l=1}^{n} d_{jl} B\psi_{l} = \sum_{l=1}^{n} \beta d_{jl} \psi_{l} \text{ or } \sum_{l=1}^{n} d_{jl} \sum_{k=1}^{n} c_{lk} \psi_{k} = \sum_{l=1}^{n} \beta d_{jl} \psi_{l}$$

$$\left\{ :: \text{ From (52), we have } B\psi_{l} = \sum_{k=1}^{n} c_{lk} \psi_{k} \right\}$$
or
$$\sum_{l,k=1}^{n} d_{jl} c_{lk} \psi_{k} = \sum_{l,k=1}^{n} \beta \delta_{lk} d_{jl} \psi_{k}$$
or
$$\sum_{l=1}^{n} (c_{lk} - \beta \delta_{lk}) d_{jl} = 0, \qquad \dots (54)$$

for k=1, 2, 3, ..., n and j fixed.

These are 'n' homogeneous linear equations in 'n' unknown d_{Il} (l=1, 2, ..., n). For a non-trivial solution of these, the determinant of the matrix of the coefficients, $[(c_{lk}-\beta \delta_{lk})]$, should vanish;

$$||c_{lk}-\beta \delta_{lk}||=0. \qquad ...(54)$$

On evaluating the determinant, we get a polynomial of degree 'n' in β , hence, it will have 'n' roots $\{\beta_1, \beta_2, ..., \beta_n\}$. Using these

values of f_i (i=1, 2, ..., n) in (53) we can calculate the coefficients d_n and hence the simultaneous eigenfunctions $\overline{\psi}$, of A and B. Clearly

$$A \overline{\psi}_{j} = A \sum_{l=1}^{n} d_{jl} \psi_{l} ; j=1, 2, ..., n = \sum_{l=1}^{n} d_{jl} A \psi_{l}$$

$$= \sum_{l=1}^{n} d_{jl} \alpha \psi_{l} \qquad \{ :: A \psi_{l} = \alpha \psi_{l} ; l=1, 2, ..., n \}$$

$$= \alpha \sum_{l=1}^{n} d_{jl} \psi_{l} = \alpha \overline{\psi}_{l}$$

and $B\overline{\psi}_j = \beta\overline{\psi}_j$ (j=1, 2, ..., n) by our demand.

Thus, if α is *n*-fold degenerate eigenvalue of A, then we can find *n*-eigenfunctions $\overline{\psi_j}$ (j=1, 2, ..., n) of B which are also the eigenfunctions of A; *i.e.*, they are the simultaneous eigenfunctions of A and B.

Thus we see that the necessary as well as sufficient condition for two dynamical variables to be measured simultaneously is that the operators corresponding to these variables must commute with each other.

2 12. UNCERTAINTY RELATION FOR OPERATORS:

In the previous section we have seen that the commuting operators have simultaneous eigenfunctions and hence the observables corresponding to such operators can be accurately and simultaneously measured. But when the operators do not commute, it is not possible to measure the dynamical variables, to which these operators correspond, accurately and simultaneously. In such a situation, the operators satisfy an uncertainty relation as shown below:

Let A and B be two Hermitian operators which do not commute;

i.e.,
$$[A, B] = iC, C \neq 0.$$
 ...(55)

Then the uncertainties $\triangle A$ and $\triangle B$ in the measurement of the classical variables corresponding to A and B, satisfy the relation

$$\triangle A. \triangle B \geqslant \frac{1}{2} \langle C \rangle.$$
 ...(56)

Here $\langle C \rangle$ is the expectation value of the operator C.

To prove the above uncertainty relation we must first define what we mean by $\triangle A$ and $\triangle B$. Although many expressions are possible, the simplest is the rootmean-square deviation from the mean, where "mean" implies the expectation value,

$$(\triangle A)^2 = \langle (A - \langle A \rangle)^2 \rangle$$

$$(\triangle B)^2 = \langle (B - \langle B \rangle)^2 \rangle.$$
(57)

Now we consider an operator

$$D = A + i\beta B$$
,

where β is an arbitrary real number. Then, the expectation value of $\frac{1}{2} \frac{1}{2} \frac{1}{2$

$$|D|^{2} = (A+i\beta B) (A\dagger - i\beta B\dagger)$$

$$= (A+i\beta B) (A-i\beta B)$$

$$\{ : A \text{ and } B \text{ are self-adjoint or Hermitian} \}$$

$$= A^{2} + \beta^{2} B^{2} - i\beta (AB - BA),$$

is given by-

$$\langle |D|^{2} \rangle = \int \psi^{*} \left[A^{2} + \beta^{2} B^{2} - i\beta \left(A\beta - BA \right) \right] \psi \, d^{3}r$$

$$= \int \psi^{*} \left(A^{2} + \beta^{2} B^{2} + \beta C \right) \psi \, d^{3}r \quad \{\text{using (55)}\}$$

$$= \langle A^{2} \rangle + \beta^{2} \langle B^{2} \rangle + \beta \langle C \rangle. \qquad ...(58)$$

Clearly, the left hand side being the expectation value of the square of the absolute value of an operator must be positive. We therefore, have from (58) that

$$\langle A^2 \rangle + \beta^2 \langle B^2 \rangle + \beta \langle C \rangle \geqslant 0.$$
 ...(59)

Now, the left hand side of the above equation is a quadratic equation in β , and the condition for a quadratic equation

$$ax^2+bx+c$$
, $= 0$

to be always positive is that the discriminant (b^2-4ac) should be negative. Thus for (59), we have

$$\langle C \rangle^2 - 4 \langle A^2 \rangle \langle B^2 \rangle \leqslant 0$$
$$\langle A^2 \rangle \langle B^2 \rangle \geqslant \frac{1}{4} \langle C \rangle^2. \tag{60}$$

or

or

If we consider a special case; $\langle A \rangle = \langle B \rangle = 0$, then from (57) and (60), we have

$$(\triangle A)^2 \cdot (\triangle B)^2 \geqslant \frac{1}{4} \langle C \rangle^2$$
$$\triangle A \cdot \triangle B \geqslant \frac{1}{2} \langle C \rangle,$$

which is the uncertainty relation, but it is true only when $\langle A \rangle = \langle B \rangle = 0$. To generalize the proof of the above relation for

the cases where $\langle A \rangle$ and $\langle B \rangle$ are non-zero, we write

$$F_1 = A - \langle A \rangle \text{ and } F_2 = B - \langle B \rangle.$$

$$\therefore [F_1, F_2] = [(A - \langle A \rangle), (B - \langle B \rangle)]$$

$$= (A - \langle A \rangle) (B - \langle B \rangle) - (B - \langle B \rangle) (A - \langle A \rangle)$$

$$= AB - A \langle B \rangle - \langle A \rangle B + \langle A \rangle \langle B \rangle - BA + B \langle A \rangle$$

$$+ \langle B \rangle A - \langle B \rangle \langle A \rangle$$

$$= AB - BA \qquad \{ \because \langle A \rangle \text{ and } \langle B \rangle \text{ are scalars} \}$$

i.e., F_1 and F_2 satisfy the same commutation relation as A and B.

Moreover,
$$\langle F_1 \rangle = \langle (A - \langle A \rangle) \rangle = \langle A \rangle - \langle A \rangle = 0$$

and $\langle F_2 \rangle = \langle (B - \langle B \rangle) \rangle = \langle B \rangle - \langle B \rangle = 0$.

Thus, from the above proof of the uncertainty for the special case $\langle A \rangle = \langle B \rangle = 0$, we have

$$\triangle F_1 \cdot \triangle F_2 \geqslant \frac{1}{2} \langle C \rangle. \qquad \dots (61)$$
Now, $(\triangle F_1)^2 = \langle (F_1 - \langle F_1 \rangle)^2 \rangle = \langle F_1^2 \rangle = \langle (A - \langle A \rangle)^2 \rangle = (\triangle A)^2$
and $(\triangle F_2)^2 = \langle (F_2 - \langle F_2 \rangle)^2 \rangle = \langle F_2^2 \rangle = \langle (B - \langle B \rangle)^2 \rangle = (\triangle B)^2.$
Hence, we have from (61),
$$\triangle A \cdot \triangle B \geqslant \frac{1}{2} \langle C \rangle.$$

This proves the uncertainty relation for the case where $\langle A \rangle$ and $\langle B \rangle$ is not necessarily zero.

2.13. THE FUNDAMENTAL COMMUTATION RELATION:

The fundamental quantities in terms of which all the dynamical observables of classical motion can be expressed, are the position coordinate ' x_c ' and the linear momentum ' p_{xc} ' along the direction of motion, which we call as the x-axis. The connection between the classical and quantum theories is given by the correspondence,

$$x_c \to x$$
; $p_{xc} \to p_x = -i\hbar \frac{\partial}{\partial x}$

where x and p_x are the quantum mechanical operators corresponding to the classical quantities x_c and p_{xc} . The commutation relation for the operators x and p_x , corresponding to the fundamental quantities of classical mechanics, is called the fundamental commutation relation. It is given by

$$[x, p_x] = i\hbar$$
 ...(62)
To prove this relation, we have for any wavefunction ψ ,

or

and
$$x p_{x} \psi = -i \hbar x \frac{\partial \psi}{\partial x}$$

$$p_{x} x \psi = -i \hbar \frac{\partial}{\partial x} (x \psi) = -i \hbar x \frac{\partial \psi}{\partial x} - i \hbar \psi$$

$$\therefore x p_{x} \psi - p_{x} x \psi = i \hbar \psi$$

 $(xp_x - p_x x) \psi = i \hbar \psi \quad \text{or} \quad [x, p_x] \psi = i \hbar \psi$ $\Rightarrow [x, p_x] = i \hbar$

Similarly, we can show that

$$[y, p_y] = [z, p_z] = i\hbar$$
 ...(63)

Relations (62) and (63) are all called as fundamental commutation relation.

2'14. CONNECTION BETWEEN THE COMMUTATOR BRACKETS AND THE POISSON BRACKETS:

Poisson bracket for any two classical dynamical observables f_c and g_c , which are the functions of x_c and p_{xc} , is defined by the equation

$$\{f_c, g_c\} = \frac{\partial f_c}{\partial x_c} \cdot \frac{\partial g_c}{\partial p_{xc}} - \frac{\partial f_c}{\partial p_{xc}} \cdot \frac{\partial g_c}{\partial x_c} \qquad \dots (64)$$

If, as a particular case we take $f_c \equiv x_c$ and $g_c \equiv p_{xc}$, then

$$\{x_c, p_{xc}\} = 1$$
 ...(65)

Also, the commutator bracket for the operators, x and p_x , corresponding to x_c and p_{xc} , is given as

$$[x, p_x] = i\hbar \qquad \dots (66)$$

Comparing (65) and (66), we can give the following relation between the Poisson bracket of x_c , p_{xc} and the commutator bracket of the corresponding operators x, p_x ,

$$i\hbar \{x_c, p_{xc}\} \rightarrow [x, p_x] \qquad \dots (67)$$

In general, if f and g are the operators corresponding to the classical functions f_o and g_c , then

$$i\hbar \{f_c, g_c\} \rightarrow [f, g] \qquad \dots (68)$$

Thus, all the identities satisfied by the Poisson brackets can be seen to be satisfied by replacing the Poisson brackets by the corresponding commutator brackets

$$\{f_c, \alpha g_c\} = \alpha \{f_c, g_c\} \rightarrow [f, \alpha g] \rightarrow \alpha [f, g];$$

$$\alpha \text{ is a constant}$$

$$\{f_c, g_c\} = -\{g_c, f_c\} \rightarrow [f, g] = -[g, f]$$

$$\{f_c, f_c\} = 0 \rightarrow [f, f] = 0$$

$$\{f_{c}, g_{c} + h_{c}\} = \{f_{c}, g_{c}\} + \{f_{c}, h_{c}\} \rightarrow [f, g + h] = [f, g] + [f, h]$$

$$\{f_{c} + g_{c}, h_{c}\} = \{f_{c}, h_{c}\} + \{g_{c}, h_{c}\} \rightarrow [f + g, h] = [f, h] + [g, h]$$

$$\{f_{c}, g_{c}, h_{c}\} = \{f_{c}, g_{c}\} h_{c} + g_{c} \{f_{c}, h_{c}\} \rightarrow [f, g h] = [f, g] h + g [f, h]$$

$$\{f_{c}, g_{c}, h_{c}\} = \{f_{c}, h_{c}\} g_{c} + f_{c} \{g_{c}, h_{c}\} \rightarrow [f g, h] = [f, h] g + f [g, h]$$

$$\{f_{c}, g_{c}, h_{c}\} + \{h_{c}, \{f_{c}, g_{c}\}\} \rightarrow [f, [g, h]] + [h, [f, g]]$$

$$+ \{g_{c}, \{h_{c}, f_{c}\} = 0$$

$$(Jacobi's Identity)$$

The above parallelism between Poisson brackets and quantum mechanical commutators allows an elegant expression of the correspondence principle and was first given by Dirac. We shall again return to this correspondence in the next section.

2.15. EQUATION OF MOTION FOR OPERATORS:

The expectation value of an operator in the state ψ is given by

$$\langle A \rangle = \int \psi^* A \psi \, d^3 r.$$

$$\therefore \frac{d \langle A \rangle}{dt} = \int \frac{\partial \psi^*}{\partial t} A \psi \, d^3 r + \int \psi^* \frac{\partial A}{\partial t} \psi \, d^3 r + \int \psi^* A \, \frac{\partial \psi}{\partial t} \, d^3 r$$

According to the correspondence (62) between the classical dynamical observables and the quantum mechanical operators, 'A' will be a function of x and p_x , and the time does not appear explicity in it. Therefore, $\frac{\partial A}{\partial t}$ will be zero and we can write

$$\frac{d\langle A\rangle}{dt} = \int \frac{\partial \psi^*}{\partial t} A\psi d^3r + \int \psi^* A \frac{\partial \psi}{\partial t} d^3r$$

From the time dependent Schroedinger equation, we have

$$\frac{\partial \psi}{\partial t} = \frac{1}{i \, \hbar} H \psi \text{ and } \frac{\partial \psi^*}{\partial t} = -\frac{1}{i \, \hbar} H \psi^*$$

Putting these values in the above equation, we get

$$\frac{d\langle A\rangle}{dt} = -\frac{1}{i\hbar} \int H\psi^* A\psi \ d^3r + \frac{1}{i\hbar} \int \psi^* AH\psi \ d^3r$$
$$= \frac{1}{i\hbar} \int \psi^* (AH - HA) \psi \ d^3r$$

:: Hamiltonian is a Hermitian Operator}

$$= \frac{1}{i \, \hbar} \langle (AH - HA) \rangle = \frac{1}{i \, \hbar} \langle [A, H] \rangle \qquad \dots (69)$$

S

We can write this in the operator form as

$$\frac{dA}{dt} = \frac{1}{i \, \hbar} \left[A, H \right]; \qquad \dots (70)$$

i.e., the time derivative of an operator 'A' is equal to the commutator of A and H multiplied by $\frac{1}{i\hbar}$. Eqn. (70) is the equation of motion for an operator 'A' and is known as the Heisenberg's Equa-From this equation we see that, if some operator commutes with the Hamiltonian, its time rate of change will be zero; i.e., the operator will be constant in time and hence it represents a constant of motion. Thus, if the operator corresponding to any quantity commutes with Hamiltonian, than that quantity will be a constant of motion.

Now we find the correspondence between the classical and the quantum theory, as was promised in the last section. In the last section we found a correspondence by which we can transit from a classical expression to a quantum mechanical expression. Here we shall discuss a correspondence by which we can get the classical limit of a quantum mechanical expression.

The eqn. (69) can be written for A=x as,

$$\frac{d\langle x\rangle}{dt} = \frac{\langle xH - Hx\rangle}{i\hbar} \qquad \dots (71)$$

Now the L.H.S. of this equation gives the classical expression for the velocity in the sense of Ehrenfest's theorem. If we wish to compare eqn. (71) with the classical expression of the velocity, we cannot simply let the operators go over into their classical analogs, because classical observables commute and we would have the R.H.S. equal to zero. Hence we must let $\hbar \to 0$ at the

$$\therefore \lim_{h \to 0} \frac{\langle xH - Hx \rangle}{i h} = \dot{x}_c = \frac{\partial H_c}{\partial p_{xc}} \qquad \dots (72-a)$$

where the R.H.S. is the expression for the velocity in the Hamiltonian formulation of the classical Mechanics.

Similarly,

Lim
$$h \to 0 \frac{\langle p_x H - H p_x \rangle}{i h} = \dot{p}_{xc} = -\frac{\partial H_c}{\partial x_c}$$
(72) are true for any H 1...(72-b)

Eqns. (72) are true for any H_c which can be expanded in the powers of x_c and p_{xc} . For example, it can very easily be verified by taking $H_c = x_c$ and $H_c = p_{xc}$ and using the fundamental commutation relation. The verification can be continued by taking $H_c = x_c^2$ and other higher powers of x_θ and $p_{x\theta}$,

$$\frac{1}{i\hbar} [p_x, x^2] = \frac{x}{i\hbar} [p_x, x] + \frac{1}{i\hbar} [p_x, x] x$$

$$= \frac{x}{i\hbar} \times -i\hbar + \frac{1}{i\hbar} \times -i\hbar x = -2x = -\frac{\partial x^2}{\partial x}.$$

This is in agreement with the classical limit (12-b) with $H_c = x_c^2$.

More generally, this type of arguments can be continued to prove that for any two functions f and g of the position and momentum, which can be expressed in the powers of x and p_x , the following relation holds good:

$$\lim_{h \to 0} \frac{\langle gf - fg \rangle}{i \, h} = \frac{\partial g_c}{\partial x_c} \frac{\partial f_c}{\partial p_{xc}} - \frac{\partial f_c}{\partial x_c} \cdot \frac{\partial g_c}{\partial p_{xc}} = \{g_c, f_c\} \qquad ... (73)$$

This relation between the commutator (gf-fg) and the Poisson bracket $\{g_c, f_c\}$ is a little more precise statement of the correspondence between the two.

From the above discussion we see that, if a quantum system has a classical analog, expectation values of operators behave in the limit $h \rightarrow 0$, like the corresponding classical quantities.

2.16. UNITARY OPERATOR:

A linear operator whose inverse and adjoint are identical is called unitary. For a unitary operator U:

$$U^{-1}=U^{\dagger}$$
 or $UU^{\dagger}=U^{\dagger}U=I$...(74)

A unitary operator may be constructed from an ordinary Hermitian operator C,

$$U = \frac{1+iC}{1-iC'}, \quad U\dagger = \frac{1-iC}{1+iC'}, \qquad UU\dagger = I. \qquad ...(75)$$

To have another construction from a Hermitian operator, we write an arbitrary unitary operator U as:

$$U = \frac{U + U^{\dagger}}{2} + i \frac{U - U^{\dagger}}{2i} = A + iB \text{ (say)},$$

$$A = \frac{U + U^{\dagger}}{2} \text{ and } B = \frac{U - U^{\dagger}}{2i}$$

$$A^{\dagger} = \left(\frac{U + U^{\dagger}}{2}\right)^{\dagger} = \frac{U^{\dagger} + U}{2} = \frac{U + U^{\dagger}}{2} = A.$$

$$B^{\dagger} = \left(\frac{U - U^{\dagger}}{2i}\right)^{\dagger} = \frac{U^{\dagger} - U}{-2i} = \frac{U - U^{\dagger}}{2i} = B;$$

and

i.e., A and B are Hermitian. Now we will show that A and B commutes with each other. For it we have

$$AB = \frac{U + U\dagger}{2} \cdot \frac{U - U\dagger}{2i} = \frac{UU - UU\dagger + U\dagger U - U\dagger U\dagger}{4i} = \frac{UU - U\dagger U\dagger}{4i}$$

 $\{:: UU\dagger=U\dagger U=I\}$

and
$$BA = \frac{U - U\dagger}{2i} \cdot \frac{U + U\dagger}{2} = \frac{UU + UU\dagger - U\dagger U - U\dagger U\dagger}{4i} = \frac{UU - U\dagger U\dagger}{4i}$$

i.e., AB=BA; A and B commutes with one-another. Hence we can find a simultaneous eigenfunction ψ for A and B,

$$A\psi = A'\psi$$
$$B\psi = B'\psi$$
;

where A' and B' are real numbers, because A and B are Hermitian.

Now,
$$U\psi = (A+iB) \psi = (A'+iB') \psi = U'\psi$$
 (say)

: the eigenvalue of
$$U$$
 is $U' = A' + iB'$(76)

Furthermore, $A^2 + B^2 = \frac{1}{4} (U + U^{\dagger})^2 - \frac{1}{4} (U - U^{\dagger})^2 = U^{\dagger}U = I$

:
$$(A^2+B^2) \psi = (A^2+B'^2) \psi = 1 \psi$$

 $\Rightarrow A'^2+B'^2=1$; i.e., $|U'|=|A'+iB'|=\sqrt{(A'^2+B'^2)}=1$.

Thus the eigenvalue of any arbitrary unitary operator U has the absolute value unity. We can, therefore, write it as:

$$U' = \exp[iC']$$
; C' is real number ...(77)

Now, if we define a Hermitian operator C, such that

$$C\psi = C'\psi$$
.

Then

exp.
$$[iC] \psi = \left(1 + iC + \frac{(iC)^2}{2!} + \dots\right) \psi$$

$$= \left(1 + iC' + \frac{(iC')^2}{2!} + \dots\right) \psi$$

$$= e^{iC'} \psi = U' \psi = U \psi \qquad \dots (78)$$

Comparing the two sides of eqn. (78),

$$U=\exp[iC]$$
; C is a Hermitian operator. ...(79)

Hence a unitary operator can be expressed in terms of a Hermitian operator by a formula like (79).

PROBLEMS

Problem 1. Show that a set of orthonormal functions is linearly independent.

Sol. Let us consider the orthonormal set of function

$$\{\psi_1, \psi_2, \psi_3, ..., \psi_{\epsilon}, ...\}$$

Now it will be linearly independent if the relation

$$C_1\psi_1+C_3\psi_2+C_3\psi_3+...+C_i\psi_i+...=0;$$
 ...(i)

is satisfied only when all the C,'s are zero.

Now to find the coefficient C_i , we take the scalar product of the above equation with ψ_i , we get

$$C_{1}(\psi_{i}, \psi_{1}) + C_{2}(\psi_{i}, \psi_{2}) + C_{3}(\psi_{i}, \psi_{3}) + \dots + C_{i}(\psi_{i}, \psi_{i}) + \dots = 0$$
or $C_{1}.0 + C_{2}.0 + C_{3}.0 + \dots + C_{i}.1 + \dots = 0$

{: the set is orthonormal}

 $\Rightarrow C_i = 0$

Similarly, all the coefficients will be zero if the relation (i) is satisfied and hence the given set will be a linearly independent set of functions.

Problem 2. If $\{u_1(x), u_2(x), ...\}$ is a complete set of orthonormal functions, then show that

$$\sum_{n=1}^{\infty} u_n^* (x') u_n (x) = \delta (x - x'),$$

where $\delta(x-x')$ is the Dirac's delta function. It is known as the closure-relation.

Sol. Let us take any arbitrary function $\psi(x)$. This can be expressed in terms of the given complete set as:

$$\psi(x) = \sum_{n=1}^{\infty} C_n u_n(x), \qquad \dots (i)$$

where,

$$C_n = \int u_n^* (x) \psi(x) dx. \qquad ...(ii)$$

Putting this value of Cn in (i) we get,

$$\psi(x) = \sum_{n=1}^{\infty} \left[\int u_n^* (x') \psi(x') dx' \right] u_n(x)$$

{: the integration variable can be changed by any other variable}

$$= \int \psi(x') \left[\sum_{n=1}^{\infty} u_n * (x') u_n(x) \right] dx' \qquad \dots \text{(iii)}$$

Also from the definition of the Dirac Delta function we have,

$$\psi(x) = \int \psi(x') \, \delta(x - x') \, dx' \qquad \dots \text{(iv)}$$

Comparing (iii) with (iv), we get the required result.

$$\sum_{n=1}^{\infty} u_n^* (x') u_n (x) = \delta (x-x').$$

Problem 3. If the eigenfunctions of an operator F forms a complete set of orthonormal functions and all the eigenvalues of F are real, then F must be Hermition.

Sol. Let ψ_i $\{i=1, 2...\}$ from a complete set of eigenfunctions of F with real eigenvalues λ_i $\{i=1, 2,...\}$; i.e.

 $F\psi_{\ell} = \lambda \psi_{\ell}$ and $\lambda_{\ell}^* = \lambda_{\ell}$...(i)

Since ψ_i $\{i=1, 2,...\}$ forms a comlete set, the arbitary state $s \psi$ and ϕ can be written as—

$$\psi = \sum_{i=1}^{\infty} C_i \psi_i \quad \text{and} \quad \phi = \sum_{j=1}^{\infty} d_j \psi_j \qquad \dots (ii)$$

$$\begin{array}{ll}
\vdots & (\psi, F\phi) = (\sum_{i=1}^{\infty} C_i \psi_i, \sum_{j=1}^{\infty} d_j F \psi_j) = (\sum_{i=1}^{\infty} C_i \psi_i, \sum_{j=1}^{\infty} d_j \lambda_j \psi_j) \\
&= \sum_{i,j=1}^{\infty} \lambda_j C_i^* d_j (\psi_i, \psi_j) = \sum_{i,j=1}^{\infty} \lambda_j C_i^* d_j \delta_{ij} \\
&= \sum_{i=1}^{\infty} \lambda_{ii} C_i^* d_i. \quad \dots (iii)
\end{array}$$

Similarly,

$$(F\psi,\phi) = (\sum_{j=1}^{\infty} C_i F\psi_i, \sum_{j=1}^{\infty} d_j \psi_i) = (\sum_{j=1}^{\infty} C_i \lambda_i \psi_i, \sum_{j=1}^{\infty} d_j \psi_j)$$

$$= \sum_{j,j=1}^{\infty} C_i^* \lambda_i^* d_j (\psi_i, \psi_j) = \sum_{i,j=1}^{\infty} \lambda_i C_i^* d_j \delta_{ij}$$

$$= \sum_{i=1}^{\infty} \lambda_i C_i^* d_i \qquad \dots (iv)$$

Form (iii) and (iv) we have,

 $(\psi, F\phi) = (F\psi, \phi)$; i.e., F is a Hermitian operator,

Problem 4. Show that the momentum of a free particle is a constant of motion.

Sol. For a free particle, potential energy V=0.

Therefore,
$$H = \frac{p^2}{2m} = -\frac{\hbar}{2m} \frac{d^2}{dx^2}$$
 {: $p = -i\hbar \frac{d}{dx}$ }

Now $pH \ \psi(x) = -i\hbar \frac{d}{dx} \left[\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} \right] = \frac{i\hbar^3}{2m} \frac{d^3\psi(x)}{dx^3}$.

and $Hp(\psi) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left[-i\hbar \frac{d\psi(x)}{dx} \right] = \frac{i\hbar^3}{2m} \frac{d^3\psi(x)}{dx^3}$.

 $pH\psi(x) - Hp\psi(x) = 0$

$$\Rightarrow pH - Hp = 0.$$

i.e. $[p, H] = 0, \gamma$

or

Thus the momentum of a free particle commutes with the Hamiltonian and hence it is a constant of motion.

Problems 5. Show that the momentum operator $p = -i\hbar \nabla_{is}$ Hermitian operator.

It the momentum operator is Hermitian, it should satisfy the equation

$$\int \psi^* \left(-i\hbar \nabla \psi\right) d^3r = \int \left(-i\hbar \nabla \psi\right)^* \psi d^3r$$
or
$$-i\hbar \int \psi^* \left(\nabla \psi\right) d^3r = i\hbar \int \left(\nabla \psi^*\right) \psi d^3r$$
Now,
$$\nabla \left(\psi^* \psi\right) = \psi^* \left(\nabla \psi\right) + \left(\nabla \psi^*\right) \psi.$$

$$\therefore \psi^* \left(\nabla \psi\right) = \nabla \left(\psi^* \psi\right) - \left(\nabla \psi^*\right) \psi.$$

Integrating this equation throughout, we get

$$\int \psi^* (\nabla \psi) d^3r = \int \nabla (\psi^* \psi) d^3r - \int (\nabla \psi^*) \psi d^3r$$

$$= \nabla \int \psi^* \psi d^3r - \int (\nabla \psi^*) \psi d^3r$$

$$= -\int (\nabla \psi^*) \psi d^3r \left\{ \therefore \int \psi^* \psi d^3r = N(\text{a consatnt}) \right\}$$

Multiplying both sides of the above equation by $-i\hbar$, we get required condition (i) and hence the momentum operater is a Hermitian operator

Problem 6.) If $=\frac{1}{2} m \dot{x}^2 + V(x)$, then show that $i\hbar\dot{x}=xH-Hx$

is satisfied if $x p_x - p_x x = ih$, where $\dot{x} = \frac{dx}{dt}$.

[Here V(x) is a potential function]

The momentum $p_x = \text{mass} \times \text{velocity} = m\dot{x}$

$$\dot{x} = \frac{p_x}{m}$$

Hence,
$$H = \frac{1}{2}m\dot{x}^2 + V(x) = \frac{1}{2}m\frac{p_x^2}{m^2} + V(x) = \frac{p_x^2}{2m} + V(x)$$
.

Now we have, $xH-Hx\equiv[x, H]$

$$= \left[x, \frac{p_x^2}{2m} + V(x) \right]$$

$$= \frac{1}{2m} \left[x, p_x^2 \right] + \left[x, V(x) \right]$$

$$= \frac{1}{2m} \left[x, p_x^2 \right]$$

 $\{: V(x) \text{ is a function of } x \text{ only and hence it will commute with } x, therefore, the second commutator bracket will vanish}$

$$\therefore xH - Hx = \frac{1}{2m} [x, p_x] p_x + \frac{1}{2m} p_x [x, p_x]$$

$$= \frac{1}{2m} \cdot i\hbar \cdot p_x + \frac{1}{2m} \cdot p_x i\hbar \{ \because [x, p_x] \equiv xp_x - p_x x = i\hbar \}$$

$$= i\hbar \frac{p_x}{m} = \frac{i\hbar}{m} m\dot{x} = i\hbar \dot{x}.$$

Problem 7. The parity operator π is defined by the operation $\pi \psi(x) = \psi(-x)$; for any function $\psi(x)$.

Show that,

- (i) It is a linear operator.
- (it) It is Hermitian operator.
- (iii) Find out the eigenvalues of this operator.
- (iv) If the potential energy is an even function, then show that π commutes with the Hamiltonian,

$$H = \frac{p^2}{2m} + V(x).$$

Sol. (i) For functions $\psi_1(x)$ and $\psi_2(x)$ we have,

$$\pi \left[\psi_1(x) + \psi_2(x) \right] = \psi_1(-x) + \psi_2(-x) = \pi \psi_1(x) + \pi \psi_2(x) \qquad \dots (i)$$

and

$$\pi [C\psi_1(x)] = C\psi_1(-x) = C\pi \psi_1(x)$$
 ...(ii)

From (i) and (ii) we see that π is a linear operator.

(ii) To show that π is Hermitian, we should be able to show that,

$$(\psi, \pi \phi) = (\pi \psi, \phi).$$

$$(\psi, \pi \phi) = \int \psi^*(x) \phi(-x) dx.$$

Now,

Since the variable of integration in an integral can be replaced by any other variable without affecting the value of the integral; by making the change of variable x'=-x, we get

$$(\psi, \pi \phi) = \int \psi^* (-x') \ \phi (x') \ dx'$$

$$= \int \psi^* (-x) \ \phi (x) \ dx$$

$$(\psi, \pi \phi) = (\pi \ \psi, \phi). \qquad \dots (iii)$$

OT

Thus m is a Hermitian operator. It should, therefore, have

real eigenvalues. $\sqrt{\text{(iii)}}$ To find the eigenvalues of π , we write the eigenvalue

equation for it as, $\pi \psi = \lambda \psi, \qquad ...(iv)$

where λ is the eigenvalue of π in the state ψ .

. Multiplying (iv) by π , we get

$$\pi^2 \psi = \lambda \pi \psi = \lambda^2 \psi$$

$$\pi^2 \psi = \lambda^2 \psi$$

or

Because the original function is restored when the transformation $x \rightarrow -x$ is performed twice. Consequently, the eigenvalues of π satisfy the equation $\lambda^2=1$, whence $\lambda=\pm 1$. The eigenfunctions belonging to the eigenvalues $\lambda = +1$ of the parity operator are the even functions ψ_{θ} , defined by

$$\psi_{e}(x) = \psi_{e}(-x). \qquad \dots (v)$$

And the eigenfunctions belonging to the eigenvalue $\lambda = -1$ are the odd functions ψ_0 , defined by

$$\psi_0(x) = -\psi_0(-x).$$

The eigenfunctions of π are a complete set w. r. t. the class of functions of x. Any functions $\psi(x)$ can be expressed as

 $\psi(x) = \frac{1}{2} \left[\psi(x) + \psi(-x) \right] + \frac{1}{2} \left[\psi(x) - \psi(-x) \right],$

where $[\psi(x) + \psi(-x)]$ is an even function of x and $[\psi(x) - \psi(-x)]$ is an odd function of x.

To show that π commutes with H, we have

$$H\psi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x)$$

$$\left\{ : p = -i\hbar \frac{d}{dx}, : p^2 = -\hbar^2 \frac{d^2}{dx^2} \right\}$$

$$\pi H\psi(x) = -\frac{\hbar^2}{2m} \pi \frac{d^2 \psi(x)}{dx^2} + \pi V(x) \psi(x)$$

$$= -\frac{\hbar^2}{2m} \frac{d^2 \psi(-x)}{dx^2} + V(-x) \psi(-x)$$

$$= -\frac{\hbar^2}{2m} \frac{d^2 \psi(-x)}{dx^2} + V(x) \psi(-x)$$

$$\{ :: V(x) \text{ is an even function} \}$$

$$= \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(-x)$$

or

and

$$\pi H \psi(x) = H \psi(-x) = H \pi \psi(x).$$

 $H\pi - \pi H = [H, \pi] = 0$; because the above equation is true for arbitrary $\psi(x)$.

Problem 8. If A and B are two operators, then show that $[A, B^{-1}] = -B^{-1}[A, B]B^{-1}.$

The right hand side of the above equation is written as $-B^{-1}[A, B]B^{-1} = -B^{-1}(AB - BA)B^{-1}$ $=-B^{-1}(ABB^{-1}-BAB^{-1})$

=
$$-B^{-1}ABB^{-1}+B^{-1}BAB^{-1}$$

= $-B^{-1}A+AB^{-1}$
{: By definition, $B^{-1}B=BB^{-1}=1$ }
= $AB^{-1}-B^{-1}A=$ left hand side.

Problem 9.) Show that the operators $(x^2p_x^2 + p_x^2x^2)$ and $(xp_x + p_x x)^2$ differ by a term of the order of h^2 .

Sol.
$$(x^{2}p_{x}^{2} + p_{x}^{2}x^{2}) - \frac{1}{2} (xp_{x} + p_{x}x)^{2}$$

$$= \frac{1}{2} \{x^{2}p_{x}^{2} + x^{2}p_{x}^{2} + p_{x}^{2}x^{2} + p_{x}^{2}x^{2} \}$$

$$- \frac{1}{2} \{xp_{x}xp_{x} + xp_{x}^{2}x + p_{x}x^{2}p_{x} + p_{x}xp_{x}x \}$$

$$= \frac{1}{2} \{(x^{2}p_{x}^{2} - xp_{x}^{2}x) + (p_{x}^{2}x^{2} - p_{x}x^{2}p_{x})$$

$$+ (x^{2}p_{x}^{2} - xp_{x}xp_{x}) + (p_{x}^{2}x^{2} - p_{x}xp_{x}x) \}$$

$$= \frac{1}{2} \{x [x, p_{x}^{2}] + p_{x} [p_{x}, x^{2}] + x [x, p_{x}] p_{x} + p_{x} [p_{x}, x] x \}$$

$$= \frac{1}{2} \{2i\hbar xp_{x} - 2i\hbar p_{x}x + i\hbar xp_{x} - i\hbar p_{x}x \}$$

$$\therefore [x, p_{x}] = i\hbar ; [p_{x}, x] = -i\hbar ;$$

$$[x, p_{x}^{2}] = [x, p_{x}] p_{x} + p_{x} [x, p_{x}] = i\hbar p_{x} + p_{x}.i\hbar = 2i\hbar p_{x},$$

$$[p_{x}, x^{2}] = x [p_{x}, x] + [p_{x}, x] x = -xi\hbar + (-i\hbar) x$$

$$= -2i\hbar x \}$$

and

 $= \frac{1}{2} \left\{ 2i\hbar \left[x, p_x \right] + i\hbar \left[x, p_x \right] \right\}$ $= \frac{3}{2} i\hbar \left[x, p_x \right] = \frac{3}{2} i\hbar .i\hbar = -\frac{3}{2} \hbar^2,$

which is of the order of ħ2.

Problem 10. By mathematical induction on n, show that $[x^n, p] = i \hbar n x^{n-1}$ and $[x, p^n] = i \hbar n p^{n-1}$, ...(i)

where n is any positive integer. Hence, prove that

$$[f(x), p] = i\hbar \frac{\partial f}{\partial x}$$
 and $[x, f(p)] = i\hbar \frac{\partial f}{\partial p}$, ...(ii)

where f(x) is any polynomial in x and f(p) is a polynomial in p.

Sol. The principle of mathematical induction states that if a relation is true for n=1, 2; and by supposing it true for n=k we can prove it for n=k+1, then it will be true for all positive integers.

Now, from the fundamental commutation relation, we have

$$[x, p] = i\hbar$$

thus the relations (i) are true for n=1.

Also, we have

 $[x^2, p] = x [x, p] + [x, p] x = x.ih + x.ih = 2ihx = ih.2x^{2-1}$ and $[x, p^2] = p [x, p] + [x, p] p = p.ih + ihp = 2ihp = ih.2p^{2-1}$.

Hence the relations (i) are true for n=2, also.

Let us now suppose that for any positive integer n=k, the relations (i) hold good,

··(iii)

i.e.,
$$[x^k, p] = i \hbar k x^{k-1}$$
 and $[x, p^k] = i \hbar k p^{k-1}$.

Then,

$$[x^{k+1}, p] = [x.x^k, p] = x [x^k, p] + [x, p] x^k$$

$$= x.i \hbar k x^{k-1} + i \hbar x^k \quad \{\text{using (iii)}\}$$

$$= i \hbar (k+1) x^{(k+1)-1} \qquad \dots (iv-a)$$

and
$$[x, p^{k+1}] = [x, p.p^k] = p[x, p^k] + [x, p] p^k$$

 $= p.i \hbar k p^{k-1} + i \hbar p^k$
 $= i \hbar (k+1) p^{(k+1)-1}$.

Equations (iv) show that the relations (i) are true for n=k+1also, if it is true for n=k. Hence by mathematical induction it is true for all positive integers n.

To prove the relations (ii), we note that any polynomial f(x)can be written as

$$f(x) = \sum_{n=0}^{k} a_n x^n.$$

Here k is the degree of the polynomial

$$\therefore \frac{\partial f(x)}{\partial x} = \sum_{n=1}^{k} n a_n x^{n-1}.$$
 ...(v)

Now we have,

$$[f(x), p] = \begin{bmatrix} \sum_{n=0}^{k} a_n x^n, p \\ \sum_{n=0}^{k} a_n x^n, p \end{bmatrix} = \sum_{n=0}^{k} a_n [x^n, p]$$

$$= i \hbar \sum_{n=1}^{k} a_n n x^{n-1} \quad \{\text{using (i)}\}$$

$$= i \hbar \frac{\partial f(x)}{\partial x}. \quad \{\text{using (v)}\}$$

Similarly, we can show by writing $f(p) = \sum_{n=0}^{k} a_n p^n$ and using

(i), that
$$[x, f(p)] = i \hbar \frac{\partial f(p)}{\partial p}$$
.

Problem 11. If $H = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2x^2$, then show that

(i)
$$xH-Hx=\frac{i\hbar}{u}p$$
.

(i)
$$xH-Hx=\frac{i\hbar}{\mu}p$$
. (ii) $pH-Hp=-i\hbar\mu\omega^2x$.

Sol. We have,

(i)
$$xH - Hx = [x, H] = \left[x, \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2\right]$$

= $\left[x, \frac{p^2}{2\mu}\right] + \left[x, \frac{1}{2} \mu \omega^2 x^2\right]$

$$[y',H] = \frac{1}{2\mu} [x, p^2] + \frac{1}{2} \mu \omega^2 [x, x^2] = \frac{1}{2\mu} [x, p^2]$$

every operator commutes with itself and hence with any power of itself}

$$=\frac{1}{2\mu}.2 i\hbar p = \frac{i\hbar}{\mu} p.$$

(ii)
$$pH-Hp = [p, H] = \left[p, \frac{p^2}{2\mu} \right] + [p, \frac{1}{2}\mu\omega^2 x^2]$$

 $= \frac{1}{2\mu} [p \cdot p^2] + \frac{1}{2}\mu\omega^2 [p, x^2]$
 $= \frac{1}{2}\mu\omega^2 [p, x^2].$
 $= \frac{1}{2}\mu\omega^2 (-2i\hbar x)$
 $\{ : [x^2, p] = 2i\hbar x, : [p, x^2] = -2i\hbar x \}$
 $= -i\hbar\mu\omega^2 x.$

Problem 12. If $H = \frac{p^2}{2m} + V(x)$, then show that

$$[x, [x, H]] = -\frac{\hbar^2}{m}.$$

Sol. We have,

$$[x, H] = \left[x, \frac{p^2}{2m}\right] + [x, V(x)].$$

Now x will commute with V(x), which is function of x; for any operator commutes with itself and hence with any of its power and any function of itself. Thus, [x, V(x)]=0 and

$$[x, H] = \left[x, \frac{p^2}{2m}\right] = \frac{1}{2m} [x, p^2] = \frac{1}{2m} \cdot 2i \, \hbar p = \frac{i \, \hbar}{m} p.$$

$$\therefore [x, [x, H]] = \left[x, \frac{i\hbar}{m} p\right] = \frac{i\hbar}{m} [x, p] = \frac{i\hbar}{m} .i\hbar = -\frac{\hbar^2}{m}.$$

Problem 13. The operators a and at are defined as

$$a = \sqrt{\left(\frac{m\omega}{2\hbar}\right)\left(x - i\frac{p}{m\omega}\right)}$$

and

$$a\dagger = \sqrt{\binom{m\omega}{2\hbar}} \left(x + i\frac{p}{m\omega}\right).$$

Find the value of $[a, a\dagger]$.

Sol.
$$[a, a\dagger] = \left[\sqrt{\left(\frac{m\omega}{2\hbar}\right)} \left(x - i\frac{p}{m\omega}\right), \sqrt{\left(\frac{m\omega}{2\hbar}\right)} \left(x + i\frac{p}{m\omega}\right) \right]$$

 $= \frac{m\omega}{2\hbar} \left[\left(x - i\frac{p}{m\omega}\right), \left(x + i\frac{p}{m\omega}\right) \right]$

$$\begin{split} &= \frac{m\omega}{2\hbar} \left[\left(x - \frac{ip}{m\omega} \right), x \right] + \frac{m\omega}{2\hbar} \left[\left(x - \frac{ip}{m\omega} \right), \frac{ip}{m\omega} \right] \\ &= \frac{m\omega}{2\hbar} \left[x, x \right] - \frac{im\omega}{2\hbar m\omega} \left[p, x \right] \\ &\quad + \frac{im\omega}{2\hbar m\omega} \left[x, p \right] - \frac{i^2 m\omega}{2\hbar m^2 \omega^2} \left[p, p \right] \\ &= 0 + \frac{-im\omega}{2\hbar m\omega} \cdot -i\hbar + \frac{im\omega}{2\hbar m\omega} \cdot i\hbar - 0 \\ &= -\frac{1}{2} - \frac{1}{2} = -1. \end{split}$$

 $[a, a^{\dagger}] = -1.$

Problem 14. If A and B are Hermitian operators, then show that i [A, B] is also Hermitian.

Sol. Let us denote the operator i [A, B] by C,

i.e.,
$$C=i [A, B]=i (AB-BA)$$
.
Then $C\dagger = -i [(AB)\dagger - (BA)\dagger]$
 $=-i [B\dagger A\dagger - A\dagger B\dagger]$
 $=-i [BA-AB]$
{:. A and B are Hermitian, therefore
 $A\dagger = A$ and $B\dagger = B$ }

=i [AB-BA]=C,

i.e. C = C and hence C is also Hermitian.

Problem 15. If A and B are two operators which commute with their commutator [A, B], prove that

(a)
$$[A, B^n] = nB^{n-1}[A, B]$$

(b) $[A^n, B] = nA^{n-1}[A, B]$...(i)

Sol. Since A and B commute with their commutator, we have

A [A, B] = [A, B] A B [A, B] = [A, B] B ...(ii)

and

It is clear that the relation (i) are true for n=1.

Also
$$[A, B^2] = [A, BB] = [A, B] B + B [A, B]$$

$$=B[A, B]+B[A, B]$$
 {using (ii)}
 $=2B^{2-1}[A, B].$

And
$$[A^2, B] = [A A, B] = A [A, B] + [A, B] A$$

= $A [A, B] + A [A, B]$ {using (ii)}
= $2A^{2-1} [A, B]$.

Hence the relations (i) are also true for x=2.

Let us now suppose that (i) is true for n=k, i.e. $[A, B^k] = kB^{k-1}[A, B]$ and $[A^k, B] = kA^{k-1}[A, B]$...(iii)

 $[A, B^{k+1}] = [A, B B^k] = B [A, B^k] + [A, B] B^k$ $=B[A, B^k]+B^k[A, B]$

[A, B] commutes with A and B, therefore, It will also commute with any powers of A and B}

$$=B.kB^{k-1}[A, B]+B^{k}[A, B]$$

$$=kB^{k}[A, B]+B^{k}[A, B]$$

$$=(k+1)B^{(k+1)-1}A, B].$$

$$[A^{k+1}, B] = [A.A^k, B] = A [A^k, B] + [A, B] A^k$$

$$= A.kA^{k-1} [A, B] + A^k [A, B]$$

$$= (k+1) A^{(k+1)-1} [A, B].$$
if

Thus the relations (i) are also true for n=(k+1), if they are true for n=k. Hence by the principle of Mathematical Induction, the relations (i) are true for all values of n.

Problem 16. Given the Hamiltonian for a charged particle in ah electromagnetic field,

$$H = \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right)^2 + e\phi(x).$$

Show that,

$$\frac{dx}{dt} = \frac{1}{m} \left(p - \frac{e}{c} A(x) \right)$$

Interprete this result in terms of its classical analog.

Sol. From the Heisenberg's equation of motion for an operator, we have

Now,
$$[x, H] = \left[x, \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right)^2 + e \phi(x) \right]$$

$$= \left[x, \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right)^2 \right] + \left[x, e \phi(x) \right]$$

$$= \left[x, \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right)^2 \right]$$

$$= \left[x, \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right)^2 \right]$$

$$\vdots \quad [x e \phi(x)] = e \left[x, \phi(x) \right] = 0, \text{ sinc}$$

 $[x, e \phi(x)] = e[x, \phi(x)] = 0$, since the scalar potential ϕ is a function of x only and hence it commutes with x; for every operator commutes with itself.}

$$= \frac{1}{2m} \left[x, \left(p - \frac{e}{c} A(x) \right) \left(p - \frac{e}{c} A(x) \right) \right]$$

$$= \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right) \left[x, \left(p - \frac{e}{c} A(x) \right) \right]$$

$$+\frac{1}{2m}\left[x,\left(p-\frac{e}{c}A(x)\right)\left(p-\frac{e}{c}A(x)\right)\right].$$
Now,
$$\left[x,\left(p-\frac{e}{c}A(x)\right)\right] = \left[x,p\right] - \frac{e}{c}\left[x,A(x)\right]$$

$$= \left[x,p\right]$$

$$\{: x \text{ commutes with } A(x), \text{ which is a function of } x \text{ only}\}$$

$$= i \ln$$

$$[x, H] = \frac{1}{2m} \left(p - \frac{e}{c} A(x) \right) . i \ln + \frac{1}{2m} . i \ln \left(p - \frac{e}{c} A(x) \right)$$

$$= \frac{i \ln}{m} \left(p - \frac{e}{e} A(x) \right)$$

Hence, we have

Now, -

$$\frac{dx}{dt} = \frac{1}{i\hbar} \cdot \frac{i\hbar}{m} \left(p - \frac{e}{c} A(x) \right) = \frac{1}{m} \left(p - \frac{e}{c} A(x) \right).$$

If we treat the 'x' and 'p' as the classical dynamical variables specifying the position and momentum of a particle in the presence of an electromagnetic field, then the above expression is exactly the classical relation between the velocity and momentum.

Problem 17. If A and B are constants of motion, then show that [A, B] is also a constant of motion.

Sol. Since A and B are constants of motion, therefore, they commute with the Hamiltonian; i.e.,

$$[A, H] = 0$$
 and $[B, H] = 0$.

$$[[A, B], H] = [(AB - BA), H]$$

= $[AB, H] - [BA, H]$
= $A[B, H] + [A, H]B - B[A, H] - [B, H]A$
= 0 (using (i)),

i.e, [A, B] commutes with the Hamiltonian and hence it is a constant of motion.

Problem 18. Show that xp_x is not self adjoint while (xp_x+p_xx) is a self adjoint operator.

Sol. Here we know that the position operator x and the momentum operator p_x are both self adjoint. Hence their product $x p_x$ can be self adjoint if they commute with each other.

But
$$[x, p_x] = i\hbar \neq 0;$$

i.e., they don't commute and hence $x p_x$ cannot be self adjoint.

Now,
$$(xp_x + p_x x)\dagger = (xp_x)\dagger + (p_x x)\dagger$$

$$= p_x \dagger x \dagger + x \dagger p_x \dagger$$

$$= p_x x + xp_x$$

$$= (xp_x + p_x x)$$

Thus the adjoint of (xp_x+p_xx) is equal to itself and hence (xp_x+p_xx) is self adjoint.

Problem 19. If A and B are linear operators and k is a scalar, show that

$$\epsilon^{kB} A e^{-kB} = A + k [B, A] + \frac{k^2}{2!} [B, [B, A]] + \frac{k^3}{3!} [B, [B, [B, A]]] + \dots$$

Sol. Let us consider the function

$$f(k) = e^{kB} A e^{-kB}.$$

$$df = B \cdot e^{kB} A e^{-kB} - e^{kB} A e^{-kB} B$$

$$= B f(k) - f(k) B$$

$$= [B, f(k)].$$

By interation of this equation, we have,

$$\frac{d^2f}{dk^2} = \left[B, \frac{df}{dk} \right] = \left[B, \left[B, f(k) \right] \right]$$

$$\frac{d^3f}{dk^3} = \left[B, \left[B, \frac{df}{dk} \right] \right] = \left[B, \left[B, \left[B, f(k) \right] \right] \right]$$

and similarly we can evaluate higher order derivatives of f(k).

Since $f(0)=e^0.A.e^0=A$, we can write the Maclaurin's series for f(k) as:

$$f(k)=A+k [B, A]+\frac{k^2}{2!}[B, [B, A]]+\frac{k^3}{3!}[B, [B, [B, A]]]+.....$$

i.e.
$$e^{kB}Ae^{-kB} = A + k[B, A] + \frac{k^2}{2!}[B, [B, A]] + \frac{k^3}{3!}[B, [B, B, A]] + ...$$

N.B. If in particular case, we take k=1, then we get

$$e^{B}Ae^{-B} = A + [B, A] + \frac{1}{2!}[B, [BA]] + \dots$$

Problem 20. If A and B are two operators which commute with their commutator, [A, B], prove the identity,

$$e^{A}e^{B}=e^{A+B+1/2}[A, B]$$

Sol. Let us consider the function

$$f(k) = e^{kA}e^{kB}e^{-k[A+B]}$$

$$\frac{df}{dk} = Ae^{kA}e^{kB}e^{-k(A+B)} + e^{kA}e^{kB}Be^{-k(A+B)}
- e^{kA}e^{kB}e^{-k(A+B)} \times (A+B) \qquad \dots (i)$$

Now,
$$e^{kA}B = \left(1 + kA + \frac{k^2A^2}{2!} + \frac{k^3A^3}{3!} + \dots\right)B$$

= $\left(B + kAB + \frac{k^2}{2!}A^2B + \frac{k^3}{3!}A^3B + \dots\right)$...(ii)

Since A and B commute with their commutator therefore,

$$[A^n, B] = nA^{n-1}[A, B]$$

or
$$A^nB = BA^n + nA^{n-1}[A, B]$$
 (see problem-15)

 $=BA^{n}+n[A, B]A^{n-1}$ (: [A, B] commutes with A)

Using this result in (ii) we get:

$$e^{kA}B = \left(B + k BA + \frac{k^2}{2!}BA^2 + \frac{k^3}{3!}BA^3 + \dots\right) + \left(k [A, B] + \frac{k^2}{2!} \cdot 2 [A, B] A + \frac{k^3}{3!} \cdot 3 [A, B] A^2 + \dots\right)$$

$$= B^{2} \left(1 + kA + \frac{k^2}{2!}A^2 + \frac{k^3}{3!}A^3 + \dots\right)$$

$$=B^{3}\left(1+kA+\frac{k^{2}}{2!}A^{2}+\frac{k^{3}}{3!}A^{3}+...\right) + k[A, B]\left(1+kA+\frac{k^{2}}{2!}A^{2}+...\right)$$

i.e., $e^{kA}B = Be^{kA} + k[A, B]e^{kA}$.

Similarly,
$$e^{kB}A = Ae^{kB} - k [A, B] e^{kB}$$
 ...(iii)

Also $Ae^{kA} = e^{kA}$ A and $Be^{kB} = e^{kB}$ B, because every operator commutes with any power of itself.

Using these results we can write (i) as:

$$\frac{df}{dk} = Ae^{kA}e^{kB}e^{-k(A+B)} + Be^{kA}e^{kB}e^{-k(A+B)} + k [A, B] e^{kA}e^{kB}e^{-k(A+B)}$$

$$-(A+B) e^{kA}e^{kB}e^{-k(A+B)}$$

$$\{ : e^{kA}e^{kB}e^{-k(A+B)} (A+B) = e^{kA}e^{kB} (A+B) e^{-k(A+B)}$$

$$= e^{kA}e^{kB} Ae^{-k(A+B)} + e^{kA}e^{kB} Be^{-k(A+B)}$$

$$= Ae^{kA}e^{kB}e^{-k(A+B)} - k [A, B] e^{kA}e^{kB}e^{-k(A+B)}$$

$$+ Be^{kA}e^{kB}e^{-k(A+B)} + k [A, B) e^{kA}e^{kB}e^{-k(A+B)}$$

$$= (A+B) e^{kA}e^{kB}e^{-k(A+B)}$$

$$\therefore \frac{df}{dk} = Af(k) + Bf(k) + k [A, B] f(k) - (A+B) f(k)$$

$$=k[A,B]f(k)$$

or
$$\frac{df}{f} = [A, B] k dk$$

Integrating both sides, we get

$$\log f = \frac{k^2}{2} [A, B]$$
 or $f(k) = e^{k^2/2} [A, B]$

or
$$e^{kA}e^{kB}e^{-k(A+B)} = e^{k^2/2} [A, B]$$

Taking k=1,

$$e^{A}e^{B}e^{-(A+B)} = e^{1/2} [A, B] \quad \text{or} \quad e^{A}e^{B} = e^{A+B+1/2} [A, B]$$

From it we see that $e^A e^B \neq e^{A+B}$ in case of operators.

$$[A, B] = 0$$
;

i.e., if the operators commutes, only then $e^A e^B = e^{A+B}$.

Problem 21. Find the commutation rule satisfied by the operators $p_{0p}=p$ and $x_{0p}=i\hbar \frac{\partial}{\partial p}$; the momentum and the position operators in the momentum representation, respectively.

Since the operators are given in the momentum, representation, the wavefunctions on which these operators operate are also the functions of the momentum p; i.e., these operators operate on the functions $\phi(p)$ in the momentum representation

Now,
$$x_{0p} p_{0p} \phi(p) = i\hbar \frac{\partial}{\partial p} (p\phi(p)) = i\hbar \left[\phi(p) + p \frac{\partial \phi}{\partial p} \right]$$

$$p_{0p}x_{0p} \phi(p) = p i \hbar \frac{\partial \phi}{\partial p}$$

$$\therefore (x_{0p} p_{0p} - p_{0p} x_{0p}) \phi(p) = i \hbar \phi(p) \Rightarrow x_{0p} p_{0p} - p_{0p} x_{0p}$$

$$= [x_{0p}, p_{0p}] = i \hbar$$

This is the commutation relation for x_{0p} and p_{p} .

Problem 22. If $H = \frac{p^2}{2m} + V(x)$ is the Hamiltonian for a onedimensional system, then show that $\dot{p} = -\frac{\partial V}{\partial x}$ and $\dot{x} = \frac{p}{m}$.

Sol. From Heisenberg's equation of motion we have,

$$\dot{p} = \frac{1}{i\hbar} [p, H] \text{ and } \dot{x} = \frac{1}{i\hbar} [x, H]$$

$$\dot{p} = \frac{1}{i\hbar} [p, \frac{p^2}{2m} + V(x)]$$

$$= \frac{1}{i\hbar} [p, \frac{p^2}{2m}] + \frac{1}{i\hbar} [p, V(x)]$$

$$= \frac{1}{i\hbar} [p, V(x)] \quad \{ : p \text{ commutes with its square, } p^2 \}$$

$$= \frac{1}{i\hbar} - i\hbar \frac{\partial V}{\partial x} \qquad \{ : [f(x), p] = i\hbar \frac{\partial f}{\partial x} \}$$

$$= \frac{\partial V}{\partial x}$$

And,
$$\dot{x} = \frac{1}{i\hbar} \left[x, \frac{p^2}{2m} + V(x) \right]$$

$$= \frac{1}{i\hbar} \left[x, \frac{p^2}{2m} \right] + \frac{1}{i\hbar} \left[x, V(x) \right]$$

$$= \frac{1}{i\hbar} \left[x, \frac{p^2}{2m} \right]$$

{ : every operator commutes with any of its functions}

$$= \frac{1}{i\hbar} \cdot \frac{1}{2m} [x, p^2]$$

$$= \frac{1}{2 im\hbar} \cdot i\hbar \cdot 2p = \frac{p}{m} \cdot \{ \because [x, p^n] = i\hbar np^{n-1} \}$$

Problem 23. Prove that an operator cannot have more than one. reciprocal.

Sol. Let us suppose that an operator A has two different reciprocals B_1 and B_2 . Then from the definition of reciprocal.

$$AB_1 = B_1 A = I$$
 ...(i)
 $AB_2 = B_2 A = I$. (ii)

and

From (i) and (ii), we have
$$AB_1 = AB_2$$
.

Multiplying both sides from left by A-1, we get

$$A^{-1}AB_1 = A^{-1}AB_2$$

$$IB_1 = IB_2$$

$$B_1 = B_2.$$

or or

Contrary to our supposition that B_1 and B_2 are different. Hence an operator cannot have more than one reciprocal.

Problem 24. Prove that the equation

$$A\psi(x) = \int_a^b G(x, x') \psi(x') dx' \qquad \dots (i)$$

defines a linear operation. G(x,x') is a given function of x, x', the same for all $\psi(x)$.

Sol Let us consider a function $\psi(x) = \psi_1(x) + \psi_2(x)$ where ψ_1 and ψ_2 are any given function of x. Then we have using (i),

$$A\{\psi_{1}(x) + \psi_{2}(x)\} = \int_{a}^{b} G(x, x') \left[\psi_{1}(x') + \psi_{2}(x')\right] dx'$$

$$= \int_{a}^{b} G(x, x') \psi_{1}(x') dx'$$

$$+ \int_{a}^{b} G(x, x') \psi_{2}(x') dx'$$

$$= A\psi_{1}(x) + A\psi_{2}(x). \qquad ...(ii)$$

Again, by considering $\psi(x) = C\psi_1(x)$, where C is a scalar constant,

$$A \{C\psi_{1}(x)\} = \int_{a}^{b} G(x, x') [C\psi_{1}(x')] dx'$$

$$= C \int_{a}^{b} G(x, x') \psi_{1}(x') dx'$$

$$= CA\psi_{1}(x).$$
(iii)

Equation (ii) and (iii) show that A is linear operator.

Problem 25. Let the operation A be defined by

$$A\psi(x) = \int_{-\infty}^{+\infty} U(x - x') \, \psi(x') \, dx',$$

where the function U(x) is the unit step function:

$$U(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

If the class of functions ψ is the class for which ψ and $\frac{d\psi}{dx}$ are integrable for $|x| \to \infty$, show that

$$A = \left\{ \frac{d}{dx} \right\}$$

Sol. To show that A is the inverse of $\frac{d}{dx}$, we should show that

$$A \cdot \frac{d}{dx} = \frac{d}{dx} \cdot A = I \qquad \dots (i)$$

Now
$$\frac{d}{dx}$$
 $A\psi(x) = \frac{d}{dx} \left[\int_{-\infty}^{+\infty} U(x-x') \, \psi(x') \, dx' \right]$

$$= \frac{d}{dx} \left[\int_{-\infty}^{x} U(x-x') \, \psi(x') \, dx' \right]$$

$$+ \int_{x}^{+\infty} U(x-x') \, \psi(x') \, dx' \right]$$

$$= \frac{d}{dx} \int_{-\infty}^{x} \psi(x') \, dx'$$

$$\{ \because \text{ by definition, } U(x-x') = 0 \text{ for } x' > x \text{ and } U(x-x') = 1 \text{ for } x' < x \}$$

$$= \psi(x)$$

$$\{ \because \psi(x) \text{ is integrable for } |x| \to \infty \}.$$

$$\mathcal{A} \frac{d\psi(x)}{dx} = \int_{-\infty}^{+\infty} U(x - x') \frac{d\psi(x')}{dx'} dx'$$

$$= \int_{-\infty}^{+\infty} U(x - x') \frac{d\psi(x')}{dx'} dx'$$

$$+ \int_{-\infty}^{+\infty} U(x - x') \frac{d\psi(x')}{dx'} dx'$$

$$= \int_{-\infty}^{x} \frac{d\psi(x')}{dx'} dx'$$

$$= \psi(x) \left\{ \therefore \frac{d\psi}{dx} \text{ is integrable for } |x| \to \infty \right\} \dots \text{(iii)}$$

From (ii) and (iii), we have

$$\frac{d}{dx} \cdot A\psi(x) = A \frac{d}{dx} \psi(x) = \psi(x).$$

$$\Rightarrow \frac{d}{dx} \cdot A = A \frac{d}{dx} = 1$$
, i.e., $A = \left(\frac{d}{dx}\right)^{-1}$

Problem 26. Calculate $\frac{dq}{dt}$ and $\frac{dp}{dt}$ for a particle whose Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 + \alpha q^3.$$

Here p and q are the momentum and position operators for the particle and satisfy the commutation relation

$$[q, p] = i\hbar$$
.

Sol. From Heisenberg's equation for an operator, we have

$$\begin{split} \frac{dq}{dt} &= \frac{1}{i\,\hbar} \, [q, \, H] = \frac{1}{i\,\hbar} \, \left[\, \dot{q}, \, \frac{p^2}{2m} + \frac{1}{2} \, m\omega^2 q^2 + \alpha q^3 \, \right] \\ &= \frac{1}{i\,\hbar . 2m} \, [q, \, p^2] + \frac{1}{2i\,\hbar} \, .m\omega^2 \, [q, \, q^2] + \frac{\alpha}{i\,\hbar} \, [q, \, q^3] \\ &= \frac{1}{i\,\hbar . 2m} \, \{ [q, \, p] \, p + p \, [q, \, p] \} \\ &= \frac{1}{i\,\hbar . 2m} \, [i\,\hbar p + p.i\,\hbar] = \frac{2i\,\hbar p}{2i\,\hbar m} = \frac{p}{m} \, . \end{split}$$

Again,

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$$\begin{split} \frac{dp}{dt} &= \frac{1}{i\hbar} [p, H] = \frac{1}{i\hbar} \left[p, \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 + \sigma q^3 \right] \\ &= \frac{1}{2i\hbar m} [p, p^2] + \frac{m\omega^2}{2i\hbar} [p, q^2] + \frac{\alpha}{i\hbar} [p, q^8] \\ &= \frac{m\omega^2}{2i\hbar} - 2i\hbar q + \frac{\alpha}{i\hbar} - 3iq^2 \left\{ :: [q^n, p] = ni\hbar q^{n^{-1}} \right\} \\ &= -m\omega^2 q - 3\alpha q^2. \end{split}$$

Problem 27. Show directly that i (p^2x-xp^2) is Hermitian. Sol. Let us write,

$$i \left(p^2 x - x p^2 \right) = A$$

or

$$A=i (p.p.x-x.p.p).$$

$$A = -i [(ppx)+-(xpp)+]$$

$$= -i [x+p+p+-p+p+x+]$$

$$= -i [xpp-ppx]$$

$$\{ : x \text{ and } p \text{ are Hermitian} \}$$

$$= -i [xp^2-p^2x] = i [p^2x-xp^2] = A.$$

Thus the operator $A = i (p^2x - xp^2)$ is Hermitian.

Problem 28. Show that every operator can be written as the combination of two operators, each of which is Hermitian.

Sol. Let A be any operator and let A^{\dagger} be its adjoint Now we can write A as:

$$A = \frac{A + A\dagger}{2} + i \frac{(A - A\dagger)}{2i} = B + iH \text{ (say)}$$

where

$$B = \frac{A + A\dagger}{2} \text{ and } H = \frac{A - A\dagger}{2i}$$

$$\text{Now } B\dagger = \frac{A\dagger + (A\dagger)\dagger}{2} = \frac{A\dagger + A}{2} = \frac{A + A\dagger}{2} = B \qquad \{ :: (A\dagger)\dagger = A \}$$

$$H\dagger = \frac{A\dagger - (A\dagger)\dagger}{-2i} = \frac{A\dagger - A}{-2i} = \frac{A - A\dagger}{2i} = H$$

and

Thus B and H are both Hermitian and A can be written in terms of those as
$$A = B + iH$$
.

Problem 29. Show that the position operator x and the momentum operator p_x satisfy the uncertainty relation.

$$\triangle x. \triangle p_x \geqslant \hbar/2.$$

Sol. We know that for operators A and B, satisfying the relation,

$$[A, B] = iC ; C \neq 0,$$

 $\triangle A, \triangle B \geqslant \frac{\langle C \rangle}{2}.$

For x and p_x , we have,

$$[x, p_x] = i \hbar$$

$$\therefore x \triangle p_x \geqslant \frac{\langle \hbar \rangle}{2}$$

$$\triangle x. \triangle p_x \geqslant \frac{\hbar}{2}$$

or

Problem 30. Show that complex conjugation is not a linear operator. Also show that the operator which associates the square of a function with the function is not linear.

The complex conjugation is defined by the operation.

$$A\psi = \psi^*$$
;

where A is the operator which when operates on any function & changes it into its complex conjugate.

Let us now consider a function $\psi = C_1\psi_1 + C_2\psi_2$, where ψ_1 and ψ_2 are given functions and C_1 and C_2 are arbitrary complex constants.

Then,

$$A\psi = A (C_1\psi_1 + C_2\psi_2) = (C_1\psi_1 + C_2\psi_2)^*$$

$$= (C_1\psi_1)^* + (C_2\psi_2)^*$$

$$= C_1^*\psi_1^* + C_2^*\psi_2^*,$$

$$A(C_1\psi_1 + C_2\psi_2) = C_1^* (A\psi_1) + C_2^* (A\psi_2). \qquad \dots$$

Clearly, it is not a linear operation. This type of operator is termed as an Antilinear Operator.

Again if A' is an operator, which associates the square of a function with the function, then

$$A'\psi(x) = \psi^{\mathfrak{g}}(x). \qquad \dots (iii)$$

Now for A' to be linear we should have, for given functions ψ_1 and ψ_2 ,

$$A'(C_1\psi_1+C_2\psi_2)=C_1(A'\psi_1)+C_2(A'\psi_2);$$
 where C_1 and C_2 are arbitrary complex numbers.

By choosing
$$\psi(x) = C_1 \psi_1 + C_2 \psi_2$$
 we have from (iii),
 $A' (C_1 \psi_1 + C_2 \psi_2) = (C_1 \psi_1 + C_2 \psi_2)^2$
 $= C_1^2 \psi_1^2 + C_2^2 \psi_2^2 + 2C_1 C_2 \psi_1 \psi_2$
 $= C_1^2 (A' \psi_1) + C_2^2 (A' \psi_2) + 2C_1 C_2 \psi_1 \psi_2$
 $\neq C_1 (A' \psi_1) + C_2 (A' \psi_2)$.

Thus A is not a linear operator.

Problem 31, Show that so far as the one dimensional motion of a particle is concerned, the function $u_{x'}(x) = \delta(x - x')$ for all real x' constitute a complete orthonormal set and that each of them is an eigenfunction of the position variable x with the eigenvalue x.

Sol. We have

$$\int x u_{x'}(x) dx = \int x \delta(x - x') dx$$

$$= x' \left\{ \therefore \int f(x) \delta(x - a) dx = f(a) \right\}$$

$$= x' \int \delta(x - x') dx \qquad \left\{ :: \int \delta(x - a) dx = 1 \right\}$$
$$= \int x' \delta(x - x') dx,$$

i.e.
$$\int x \, u_{x'}(x) \, dx = \int x' \, u_{x'}(x) \, dx$$
. ...(i)

Comparing both sides of the equation (i), we get,

$$x u_{x'}(x) = x' u_{x'}(x)$$
 ...(ii)

Thus $u_{x'}(x)$ is an eigenfunction of the position variable x with the eigenvalue x'.

Here the eigenvalues constitute a continuous set, hence the orthonormality condition is satisfied in the form of Dirac Delta function, instead of the Kronecker delta;

i.e.,
$$\int u_{x'}(x) \ u_{x''}(x) \ dx = \delta(x' - x'') \qquad ...(iii)$$
Now,
$$\int u_{x'}(x) \ u_{x''}(x) \ dx = \int \delta(x - x') \ \delta(x - x'') \ dx = \delta(x' - x^*)$$

$$\left\{ :: \int \delta(x - a) \ \delta(x - b) \ dx = \delta(a - b) \right\} = 0$$

Thus $u_{x'}(x)$ constitute an orthonormal set.

To prove the completeness of the set of functions $u_{x'}(x)$, let us consider any given function $\psi(x)$. Then we write,

$$\psi(x) = \int C(x') u_{x'}(x) dx'; \dots (iv)$$

where C(x') are analogous to the coefficients of expansion C_i 's in case of discrete eigenvalues [see equation (27)]. Also, the completeness condition of eqn. (36), here becomes,

$$\int \psi^{*}(x) \, \psi(x) \, dx = \int C^{*}(x') \, C(x') \, dx' \qquad \dots(v)$$
Now,
$$\int \psi^{*}(x) \, \psi(x) \, dx = \int \left(\int C(x') \, u_{x'}(x) \, dx' \right)^{*}$$

$$\left(\int C(x'') \, u_{x''}(x) \, dx'' \right) dx$$

$$= \int \int C^{*}(x') \, C(x'') \, \delta(x-x') \, \delta(x-x'') \, dx \, dx' \, dx''$$

$$= \int \int C^{*}(x') \, C(x'') \, \delta(x'-x'') \, dx' \, dx''$$

$$= \int C^* (x') C(x') dx'$$

which is the completeness relation and hence the given set of functions is complete also.

Problem 32. If A commutes with B and C commutes with B, then show that A and C may or may not commute.

Sol. Since A and C commute with B, therefore.

$$[A, B] = 0$$
 or $AB = BA$...(i)

and

$$[C, B] = 0$$
 or $CB = BC$...(ii)

Now

$$[A, C] = AC - CA. \qquad \dots (iii)$$

From (i), and (ii) we cannot say, whether (iii) will vanish. It may or may not vanish. Thus A and C may or may not commute.

Problem 33. Establish the operator equation

$$\frac{\partial}{\partial x} \cdot x^n = nx^{n-1} + x^n \frac{\partial}{\partial x}$$

and hence show that $\left[\frac{\partial}{\partial x}.x^n\right] = nx^{n-1}$.

Sol. Let us operate $\frac{\partial}{\partial x} x^n$ on any function $\psi(x)$, then

$$\frac{\partial}{\partial x} \left[x^n \psi(x) \right] = x^n \frac{\partial \psi(x)}{\partial x} + nx^{n-1} \psi(x),$$

$$\Rightarrow \frac{\partial}{\partial x} \cdot x^n = nx^{n-1} + x^n \frac{\partial}{\partial x}$$

Now,
$$\left[\frac{\partial}{\partial x}, x^n\right] = \frac{\partial}{\partial x} x^n - x^n \frac{\partial}{\partial x}$$

= $nx^{n-1} + x^n \frac{\partial}{\partial x} - x^n \frac{\partial}{\partial x} = nx^{n-1}$.

Problem 34. Show that $u(x)=e^{-\frac{1}{2}x^2}$ is an eigenfunction of the operator

$$A = \left(\frac{\partial^2}{\partial x^2} - x^2\right).$$

What is its eigenvalue?

Sol. We have,

$$Au(x) = \left(\frac{\partial^{2}}{\partial x^{2}} - x^{2}\right) e^{-\frac{1}{2}x^{2}} = \frac{\partial^{2}}{\partial x^{2}} \left(e^{-\frac{1}{2}x^{2}}\right) - x^{2}e^{-\frac{1}{2}x^{2}}$$

$$= x^{2}e^{-\frac{1}{2}x^{2}} - e^{-\frac{1}{2}x^{2}} - e^{-\frac{1}{2}x^{2}} = -e^{-\frac{1}{2}x^{2}}$$

$$= -1 \ u(x).$$

This u(x) is an eigenfunction of A with an eigenvalue -1.

Problem 35. Consider the products ABC, ACB, BCA, BAC, CAB and CBA of operators A, B and C. How many of these products are different operators (a) if no two of the A, B and C commute, (b) if A and B commute with each other, but neither A nor B commute with C, (c) if every two of the three operators commute.

Sol. (a) In this case all the products will be different.

(b) When A and B commute, then ABC=BAC and CAB=CBA

Thus only four of the products are different.

(c) In this case,

$$ACB = ABC$$
 (: $C \& B \text{ commute}$)
 $BCA = BAC$ (: $C \& A \text{ commute}$)
 $=ABC$ (: $A \& B \text{ commute}$)

Similarly, using the commuting property we see that

$$BAC = CAB = CBA = ABC$$

Thus all the products are equal to ABC.

Problem 36. Show that p^n is Hermitian operator and hence $f(p) = \sum c_n p^n$,

is also Hermitian, provided that the c_n are real. Show that if any of the c_n 's is complex, f(p), is not Hermitian.

Sol. We have shown that the momentum operator p is Hermitian, therefore,

Now
$$p^{\uparrow}=p$$
,
 $p^{n}=(p.p.p. \dots n \text{ times})$
 $p^{n}=(p.p.p. \dots n \text{ times})$

Hence p^n is Hermitian.

Now,
$$(f(p)) = (\sum_{n} c_{n} p^{n}) = \sum_{n} (c_{n} p^{n}) = \sum_{n} (c_{n} p^{n}) = \sum_{n} c_{n} p^{n} + (\text{if all the } c_{n} \text{ are real})$$

$$= \sum_{n} c_{n} p^{n} + (\text{if all the } c_{n} \text{ is Hermitian}) = f(p)$$

Thus f(p) is Hermitian.

If any of the c_n 's, say c_k , is complex, then we have $(f(p))^{\dagger} = (c_0 + c_1 p + c_2 p^2 + ... + c_k p^k + ... + c_n p^n + ...)^{\dagger}$ $= c_0 + c_1 p + c_2 (p^2)^{\dagger} + ... + c_k^* (p^k)^{\dagger} + ... + c_n (p^n)^{\dagger} + ...$ $= c_0 + c_1 p + c_2 p^2 + ... + c_k^* p^k + ... + c_n p^n + ... \neq f(p)$ $(c_k^* \neq c_k^* \neq c_k^*)$

OPERATORS IN QUANTUM MECHANICS

Hence f(p) is not Hermitian if any of the c_n 's is complex.

Problem 37. The translation operator is defined to be such that $D_{\xi} \psi(x) = \psi(x+\xi)$;

i.e., the effect of D_{ξ} is to shift the coordinate by a constant distance ξ . Show that:

- (a) D_{ξ} can be expressed interms of the operator $p = -i\hbar \frac{d}{dx}$.
- (b) D_{ξ} is unitary.

Sol. (a) Using Taylor's theorem, we can write

$$D_{\xi} \psi(n) = \psi (x + \xi) = \sum_{n=0}^{\infty} \frac{\xi^{n}}{n!} \frac{d^{n} \psi (x)}{dx^{n}}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\xi p}{\hbar} \right)^{n} \psi (x)$$

$$\left\{ \because p = \frac{\hbar}{i} \frac{d}{dx} \text{ therefore } \left(\frac{ip}{\hbar} \right)^{n} = \frac{d^{n}}{dx^{n}} \right\}$$

$$= e^{i\xi p/\hbar} \psi (x)$$

$$\Rightarrow D_{\xi} = e^{i\xi p/\hbar} \qquad \dots (ii)$$

 $\Rightarrow D_{\xi} = e \qquad ...(ii)$ (b) For any two functions $\psi(x)$ and $\phi(x)$, we define $D_{\xi} \uparrow$ by: $\int \psi^*(x) D_{\xi} \uparrow \phi(x) dx = \int (D_{\xi} \psi(x)^* \phi(x) dx)$

$$\therefore \quad \int \psi^*(x) \ D_{\xi}^{\dagger} \phi(x) \ dx = \int \psi^*(x+\xi) \phi(x) \ dx$$

By making the change of variable $x+\xi \rightarrow x$ in R.H.S. integral we get

$$\int \psi^{*}(x) D_{\xi} \dagger \phi(x) dx = \int \psi^{*}(x) \psi(x - \xi) dx,$$

$$\Rightarrow D_{\xi} \dagger \phi(x) = \phi(x - \xi)$$

$$\therefore D_{\xi} D_{\xi} \dagger \phi(x) = D_{\xi} \phi(x - \xi) = \phi(x - \xi + \xi) = \phi(x) \Rightarrow D_{\xi} D_{\xi} \dagger = I$$
Also, $D_{\xi} \dagger D_{\xi} \phi(x) = D_{\xi} \dagger \phi(x + \xi) = \phi(x + \xi - \xi) = \psi(x) \Rightarrow D_{\xi} \dagger D_{\xi} = I$

$$\therefore D_{\xi} D_{\xi} \dagger = D_{\xi} \dagger D_{\xi} = I. \text{ Hence } D_{\xi} \text{ is unitary.}$$

Problem 38. Let H(x) be an operator acting on the wavefunction $\psi(x)$, and be a coordinate transformation operator which acts on the wavefunctions in such a way that $A\psi(x)=\psi(x')$. Show that if H(x) is invariant under the coordinate transformation A; i.e., H(x')=H(x), then [H,A]=0.

Sol.
$$A(H(x) \psi(x)) = H(x') \psi(x') = H(x) \psi(x') = H(x) A \psi(x)$$

 $\Rightarrow AH(x) - H(x) A = 0$
or $[H(x), A] = 0$

Problem 39. Find the expansion of the operator $(A-\lambda B)^{-1}$ in a power series in λ , assuming that the inverse A^{-1} of A exists.

Sol. Let the power series expansion we are seeking be written as

$$(A-\lambda B)^{-1} = \sum_{n=0}^{\infty} L_n \lambda^n \qquad ...(i)$$

in which the operators L_n are to be determined.

Multiplying (i) throughout, by $(A-\lambda B)$, we obtain

$$I = \sum_{n=0}^{\infty} (A - \lambda B) L_n \lambda^n$$

or

$$I = AL_0 + \sum_{n=0}^{\infty} (AL_n - BL_{n-1}) \lambda^n \qquad \dots (ii)$$

Equating the coefficients of various powers of λ in (ii), we get

$$AL_0 = I \Rightarrow L_0 = A^{-1}$$

$$AL_n - BL_{n-1} = 0$$
 for $n = 1, 2,$

$$\Rightarrow L_n = A^{-1} BL_{n-1} \text{ for } n=1, 2, \dots$$

$$\therefore L_4 = A^{-1} B L_0 = A^{-1} B A^{-1}$$

$$L_2 = A^{-1} BL_1 = A^{-1} BA^{-1} BA^{-1}$$
; etc. etc.

So we can write,

$$(A-\lambda B)^{-1}=A^{-1}+\lambda A^{-1} BA^{-1}+\lambda^2 A^{-1} BA^{-1} BA^{-1}+\dots$$

Problem 40. The derivative of an operator $A(\lambda)$ which depends explicitly on a parameter λ is defined as:

$$\frac{dA(\lambda)}{d\lambda} = \lim_{\epsilon \to 0} \frac{A(\lambda + \epsilon) - A(\lambda)}{\epsilon}.$$

Show that,

$$\frac{d(AB)}{d\lambda} = \frac{dA}{d\lambda} B + A \frac{dB}{d\lambda}$$
 ...(i)

and.

λ,

$$\frac{d(A^{-1})}{d\lambda} = -A^{-1}\frac{dA}{d\lambda}A^{-1}.$$
 ...(ii)

Sol. We can write

$$\frac{d(AB)}{d\lambda} = \lim_{\epsilon \to 0} \frac{A(\lambda + \epsilon) B(\lambda + \epsilon) - A(\lambda) B(\lambda)}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{A(\lambda + \epsilon) B(\lambda + \epsilon) - A(\lambda + \epsilon) B(\lambda) + A(\lambda + \epsilon) B(\lambda) - A(\lambda) B(\lambda)}{\epsilon}$$

$$=\lim_{\epsilon \to 0} \frac{A(\lambda+\epsilon) \left[B(\lambda+\epsilon) - B(\lambda)\right]}{\epsilon} + \lim_{\epsilon \to 0} \frac{\left[A(\lambda+\epsilon) - A(\lambda)\right] B(\lambda)}{\delta}$$

$$=A\frac{dB}{d\lambda}+\frac{dA}{d\lambda}B.$$

To prove the equation (ii), let us differentiate $AA^{-1}=I$ w.r.t.

$$\frac{dA}{d\lambda} A^{-1} + A \frac{dA^{-1}}{d\lambda} = 0$$
i.e.,
$$A \frac{dA^{-1}}{d\lambda} = -\frac{dA}{d\lambda} A^{-1}.$$

Multiplying both sides from the left by A^{-1} we obtain

$$\frac{dA^{-1}}{d\lambda} = -A^{-1} \frac{dA}{d\lambda} A^{-1}.$$

Problem 41. Verify the identity,

$$[A, e^{-\beta B}] = e^{-\beta B} \int_0^\beta e^{\lambda B} [A, B] e^{-\lambda B} d\lambda. \qquad \dots (i)$$

where A and B are any two operators.

(Kubo's Identity)

Sol. Let us denote the left-hand side and the right-hand side of (i) by $C(\beta)$ and $D(\beta)$; respectively.

Then,
$$C(0)=D(0)=0$$
. ...(ii)

If we can also show that $C(\beta)$ and $D(\beta)$ satisfy the same first order differential equation, then the identity is valid. This is in fact the case, since

$$\frac{dC(\beta)}{d\beta} = -AHe^{-\beta H} + He^{-\beta H} A = H (e^{-\beta H}A - Ae^{-\beta H}) - (AH - HA) e^{-\beta H}$$

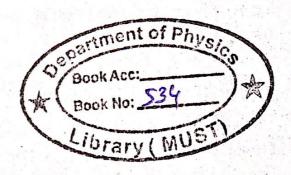
$$= H C(\beta) - [A, H] e^{-\beta H} ...(iii)$$

and

$$\frac{d D(\beta)}{d\beta} = HD - e^{-\beta H} - e^{\beta H} e^{\beta H} [A, H] e^{-\beta H}$$

$$= HD - [A, H] e^{-\beta H} \qquad \dots (iv)$$

From eqns. (iii) and (iv) we see that $C(\beta)$ and $D(\beta)$ satisfy the same differential equations with the same initial conditions (ii). Hence they are identical.



In the first two chapters we have discussed the theory of quantum mechanics developed by Schroedinger. In that formulation we have included differential operators and differential equations. We shall now describe an equivalent formulation in terms of matrices. It was historically the first formulation of quantum mechanics to be discovered by Heisenberg, Born and Jordan. But we shall deduce it from the Schroedinger approach, discussed already. In the matrix theory of quantum mechanics, dynamical variables, such as the coordinates, momentum and energy etc., appear explicitly without their being operated on a wavefunction, and hence, provides a closer resemblance with the classical theory. Two start with we recall a few elementary ideas about the vector spaces.

3.1-a. LINEAR VECTOR SPACE:

A non-empty set $V=\{u, v, w, ...\}$ is said to be a linear vector space if there are two operations called 'vector addition' and scalar multiplication' defined on V; i.e.,

- (a) For every pair $u, v \in V$, there exists an element w = u + v in V, called the sum of u and v (vector addition).
- (b) For every element $u \in V$ and every scalar α , there exists an element $\alpha.u$ in V, called the scalar multiplication of u by the scalar α , and these two operations satisfy the following properties:
 - (i) u+v=v+u; for all $u, v \in V$.
 - (ii) (u+v)+w=u+(v+w); for all $u, v, w \in V$.
- (iii) There is an element $0 \in V$, called the zero vector, such that

$$0+u=u+0=u$$
; for all $u \in V$.

(iv) Given any $u \in V$, there exists an element $-u \in V$ called the negative of u, such that

$$u+(-u)=(-u)+u=0.$$

(v) $(\alpha+\beta)u=\alpha u+\beta u$ for all $u\in V$ and any scalar α and β .

- (vi) $\alpha(u+v) = \alpha u + \alpha v$ for $u, v \in V$ and α any scalar.
- (vii) $(\alpha\beta)u=\alpha$ (βu) for $u\in V$ any scalars α and β .
- (viii) 0.u=0 for any $u \in V$.
- (ix) 1.u = u for any $u \in V$.

The set 'F' of all scalars for which the above properties are satisfied by the elements of set V is called a field and we say that the set V is a vector space over the field F.

The elements of a vector space are called vectors, though they may not be vector quantities physically. For example, the set 'C' of all complex numbers forms a vector space over the field R, the set of all real numbers. Clearly, the sum of two complex numbers is a complex number is a complex number and the product of a real number by a complex number is also complex. Thus the 'vector addition' and 'scalar multiplication' are defined on the set C, and hence, it forms a vector space. It can very easily be verified that the properties (i) to (ix) are satisfied by the set of complex numbers.

3·1-b. DIRECT PRODUCT AND DIRECT SUM OF VECTOR SPACES:

Let V_1 and V_2 be two distinct vector spaces

$$V_1 = \{u_1, v_1, w_1, \ldots\}$$

$$V_2 = \{u_2, v_2, w_2, \ldots\}$$

Then the vector space obtained by multiplying each element of V_1 by every element of V_2 is called the direct product of V_1 with V_2 . It is denoted as:

$$V \sim V_1 \otimes V_2 = \{u_1 u_2, u_1 v_2, \dots; v_1 u_2, v_1 v_2, \dots; \dots\}$$

The vector space obtained by the union of the sets V_1 and V_2 is known as the direct sum of V_1 and V_2 . It is written as:

$$V=V_1 \oplus V_2=\{u_1, v_1, w_1, ..., u_2, v_2, w_2, ...\}.$$

3·1-c. LINEAR DEPENDENCE OF VECTORS:

It is clear from the definition of vector space that for the vectors $u, v \in V$ and scalars α and β , $\alpha u + \beta v$ also belongs to V. Generalizing it, we can say that for $u_1, u_2, u_3, ..., u_n \in V$ and scalars $\alpha_1, \alpha_2, \alpha_3, ..., \alpha_n$;

$$u = \alpha_1 u_1 + \alpha_2 u_2 + \alpha_3 u_3 + \ldots + \alpha_n u_n \in V \qquad \ldots (1)$$

Vector u, defined by eqn. (1) is the linear combination of u_1 , u_2 , u_3 , ..., n_n .

The zero vector '0' can always be written as a linear combination of any finite set of vectors as

$$0 = 0.u_1 + 0.u_2 + 0.u_3 + \dots + 0.u_n \qquad \dots (2)$$

For some vectors $u_1, u_2, u_3, ..., u_n$ it may be possible that

$$0 = \alpha_1 u_1 + \alpha_2 u_2 + \alpha_3 u_3 + \ldots + \alpha_n u_n ; \qquad \ldots (3)$$

where all the $\alpha_1, \alpha_2, \ldots, \alpha_n$ are not zero. If the null vector can be expressed like (3) then the vectors $u_1, u_2, u_3, ..., u_n$ are called as linearly dependent. On the other hand, if no such linear combination exists, we say that $u_1, u_2, \dots u_n$ are linearly independent. If the vectors are linearly independent then the null vector can be expressed like (2) only.

3·1-d. DIMENSIONALITY OF A VECTOR SPACE:

A set of linearly independent vectors $\{u_1, u_2, ..., u_n\}$ in a vector space V, such that every vector of the vector space can be expressed as a linear combination of $u_1, u_2, ..., u_n$; is called a basis for the space V and the vectors $u_1, u_2, ..., u_n$ are called as spanning the space V. The number of basis vectors of a vector space is the dimensionality of the vector space. If this number is finite, we have a finite dimensional space and if it is infinity, we have an infinite dimensional space.

We are well familiar with the Eucledian space. It is a three dimensional vector space because there are only three linearly independent vectors \hat{i} , \hat{j} and \hat{k} (the unit vectors along the x, y and z direction, respectively). Any other vector of the space can readily be written as a linear combination of these

$$\mathbf{A} = A_1 \hat{\mathbf{i}} + A_2 \hat{\mathbf{j}} + A_3 \hat{\mathbf{k}}$$

We have defined the direct producr of two vector spaces V_1 and V_2 . Regarding the dimensionality of the direct product space, if n_1 and n_2 are the dimensions of V_1 and V_2 ; respectively, then $V_1 \otimes$ V_2 will be a $(n_1 \times n_2)$ dimensional space. The direct sum space $V_1 \oplus$ V_2 will be a (n_1+n_2) dimensional space.

ORTHONORMAL VECTORS:

With every ordered pair of vectors u and v in a vector space V, there is associated a scalar denoted by (u, v), which is called the scalar product of u and v and satisfies the following properties:

- (i) $(u, v) = (v, u)^*$
- (ii) $(\alpha u, \beta v) = \alpha^* \beta(u, v)$
- (iii) $(u, \alpha v + \beta w) = \alpha (u, v) + \beta (u, w)$

(iv) $(u, u) \geqslant 0$

(v)
$$(u, u)=0$$
 if and only if $u=0$.

In the above, asterisk denotes the complex conjugate. Two vectors whose scalar product is zero are said to be orthogonal.

The positive square root of the scalar product of a vector with itself, $\sqrt{[(u, u)]}$, is called the *norm* of u. If the norm of a vector is unity, it is called a unit-vector or a normalized vector. If two vectors are normalized and orthogonal also, we shall call them orthonormal vectors.

3.1-f. SCHMIDT'S ORTHOGONALIZATION METHOD:

An *n*-dimensional vector space is spanned by a set $\{u_1, u_2, ..., u_n\}$, of 'n' linearly independent vectors which are not necessarily orthonormal. But we can construct a set $\{w_1, w_2, ..., w_n\}$, of 'n' linearly indedendent orthonormal vectors, the elements w_i $(1 \le i \le n)$ of which are linear combinations of u_i $(1 \le i \le n)$. We proceed along the following steps:

(i) Let $v_1 = u_1$

1/3

and (ii) $v_2=u_2+a_{21}v_1$; where a_{21} is a constant to be determined from the condition that v_2 is orthogonal to v_1 i.e. $(v_1 \cdot v_2)=0$.

Hence we have,

$$(v_1, u_2) + a_{21} (v_1, v_1) = 0$$

$$\Rightarrow a_{21} = -\frac{(v_1, u_2)}{(v_1, v_1)}$$

Thus we have two orthogonal vectors v_1 and v_2 .

(iii) Take $v_3 = u_3 + a_{32}v_2 + a_{31}v_1$;

where a_{31} and a_{32} are constants to be determined from the condition that v_3 is orthogonal to v_1 and v_2 . This gives,

$$(v_1, v_3) = 0 = (v_1, u_3) + a_{31}(v_1, v_1) \Rightarrow a_{31} = \frac{-(v_1, u_3)}{(v_1, v_1)}$$
and $(v_2, v_3) = 0 = (v_2, u_3) + a_{32}(v_2, v_2) \Rightarrow a_{32} = \frac{(-v_2, u_3)}{(v_2, v_2)}$

Now we have three mutually orthogonal vectors v_1 , v_2 and v_3 .

This procedure can be continued and we can get 'n' orthogonal vectors v_i ($1 \le i \le n$). Finally we can normalize these by dividing with their norms and can get $\{w_1, w_2, ..., w_n\}$, of 'n' orthogonal as well as normalized vectors,

$$w_i = \frac{v_i}{\sqrt{[(v_i, v_i)]}}; 1 \leqslant i \leqslant n$$

3.2. HILBERT SPACE:

The Hilbert space is a vector space spanned by orthonormal set of basis vectors endowed with an extra property of completeness. We call an orthonormal set as complete if it is not contained in any larger orthonormal set. If we take any bigger set, the elements of that must be linearly dependent of the complete orthonormal set of basis vectors can be expressed as a linear combination of the basis vectors.

We have seen that any arbitrary quantum mechanical wavefunction, $\psi(x)$, can be written in terms of a complete set of orthronormal eigenfunctions ψ_i (i=1, 2, 3, ...) as

$$\psi(x) = \sum_{i=1}^{\infty} C_i \psi_i$$

$$C_i = (\psi_i, \psi)$$
...(4)

where

The wavefunction $\psi(x)$ is completely specified if all the C_i 's are known. We can write these in a column vector as:

$$\psi(x) = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_i \end{pmatrix} \dots (5)$$

Thus a statefunction can be represented by a column vector in an infinite dimensional space by imagining an axis for each function ψ_i , and C_i corresponds to the component of the vector in the direction of that axis. This infinite dimensional vector space spanned by the basis vectors ψ_i (i=1, 2, 3, ...) is a Hilbert space. As the statefunctions in this space are represented by column vectors, we may specifically call them as state-vectors.

3.3. DIRAC'S BRA AND KET NOTATIONS, DUAL VECTORS:

In dealing with vectors with complex scalar products we have had to be careful about the order of factors and complex conjugation. The scalar product of two state-vectors ψ_m and ψ_n has been defined as,

$$(\psi_m, \psi_n) = \int \psi_m^* \psi_n \ d^3r$$

$$(\psi_n, \psi_m) = \int \psi_n^* \psi_m \ d^3r = (\psi_m, \psi_n)^*$$

while,

Thus we see that $(\psi_m, \psi_n) \neq (\psi_n, \psi_m)$ in general, and the order

of the two factors in the scalar product is very important. Further, we have

while,
$$\begin{aligned} (\psi_m, C\psi_n) &= C \ (\psi_m, \psi_n) \\ (C\psi_m, \psi_n) &= C^* \ (\psi_m, \psi_n) \end{aligned} ;$$

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and

i.e., the scalar product is linear with respect to the post-factor while it depends on the prefactor in an antilinear fashion. To elucidate this distinction, Dirac introduced two very elegant notations, called the "Bra" and the "ket". He considered all possible state-vectors ψ in the Hilbert space (with column matrices as representatives) and denoted the typical vector by the symbol $|\rangle$, called a "ket". Into the ket $|\rangle$ may be inserted symbols denoting eigenvalues, quantum numbers, etc., which specify the state in question. All the ket vectors of a system together form a linear vector space which may be called as the ket-space.

The scalar product of any two state-vectors ψ_m and ψ_n denoted by the kets $|\psi_m\rangle$ and $|\psi_n\rangle$, is written as

$$(\psi_m, \psi_n) = \langle \psi_m \mid \psi_n \rangle ; \qquad \dots (6)$$

where the symbol $\langle \psi_m |$ is called the "bra" vector corresponding to the ket vector $|\psi_m\rangle$. Since the first three and the last three letters of BRA (C) KET provide the designation of the $\langle |$ -vector as a BRA and the $| \rangle$ -vector as a KET, this somewhat whimsical terminology is due to Dirac.

Thus we see that the "Bra" and "ket" notations distinguish very clearly the pre-factor and the post-factor wave-vectors in a scalar product. Merely writing ψ_m or ψ_n we cannot know whether it is to be the pre-factor or the post-factor, but writing $\langle \psi_m |$ and $|\psi_n \rangle$ clearly tells that ψ_m will be a pre-factor and ψ_n will be a post-factor. We assume that to every "ket" $|\rangle$, there corresponds a "bra" $\langle |$ and vice-versa, subjected to the condition:

$$\begin{array}{c|c} |1\rangle + |2\rangle \longleftrightarrow \langle 1| + \langle 2| \\ C| \rangle \longleftrightarrow C^* \langle | \end{array} ...(7)$$

where the double arrows indicate the correspondence between the two notations. All the bra vectors of a system also form a linear vector space called the bra-space. Thus the bra-space is a Dual-Space to the ket space and hence the "bra \(\) are called dual vectors. Each of the ket and the bra-spaces are linear in itself, but they are related to each other in an anti-linear manner as is seen from (7).

Operation on a ket vector from the left with an operator A produces another ket vector,

$$A \mid \psi \rangle = \mid \psi' \rangle, \qquad ...(8)$$

and the operation on a bra-vector from the right with an operator A produces another bra-vector,

$$\langle \psi \mid A = \langle \psi' \mid ...(9)$$

The expectation value of any operator A in the state ψ can be written in these notations as,

$$\langle A \rangle = \int \psi^* \ A\psi \ d^3r = \int \psi^* \ \psi' \ d^3r = \langle \psi \mid \psi' \rangle = \langle \psi \mid A \mid \psi \rangle, \quad \dots (10)$$

Now we consider the eigenvalue problem for the quantum mechanical states in these notations. If an operator 'A' operates on a ket $|\psi\rangle$ from left and

$$A \mid \psi \rangle = \lambda \mid \psi \rangle,$$
 ...(11)

then the ket $|\psi\rangle$ is called an eigenket of the operator A and λ is its eigenvalue. It is customary to represent an eigenket by its eigenvalue enclosed in a ket $|\rangle$. Thus $|\psi\rangle \equiv |\lambda\rangle$.

In these notations, the set of eigenkets

$$\{|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_n\rangle, ..., |\psi_m\rangle, ...\}$$

will be an orthonormal set of eigenkets, if

$$\langle \psi_n | \psi_m \rangle = \delta_{nm} ; n, m=1, 2, 3, ...$$
 ...(12)

If we have a complete set of eigenkets $|\psi_i\rangle$ (i=1, 2, 3, ...), then in analogy with the complete set of eigenfunctions, we can express any arbitrary ket $|\psi\rangle$ as

$$| \psi \rangle = \sum_{i=1}^{\infty} C_i | \psi_i \rangle$$

$$C_i = \langle \psi_i | \psi \rangle.$$
(13)

where

Substituting the values of C_i , we can write

$$| \psi \rangle = \sum_{i=1}^{\infty} \langle \psi_i | \psi \rangle | \psi_i \rangle = \sum_{i=1}^{\infty} | \psi_i \rangle \langle \psi_i | \psi \rangle.$$

If we take $|\psi\rangle = |\psi_i\rangle$, then

$$|\psi_{i}\rangle = \sum_{i=1}^{\infty} |\psi_{i}\rangle \langle \psi_{i} | \psi_{i}\rangle \Rightarrow \sum_{i=1}^{\infty} |\psi_{i}\rangle \langle \psi_{i} | = I.$$

Thus $\sum_{i=1}^{\infty} |\psi_i\rangle \langle \psi_i|$ is equal to unity or identity operator. It is a linear operator.

We now define an aperator P_i called the *Projection Operator* as,

$$P_i = |\psi_i\rangle \langle \psi_i|; \qquad \dots (14)$$

Clearly,
$$\sum_{i=1}^{\infty} P_i = I$$
. ...(15)

The term projection operator, reasonably so, since it projects out the part of the arbitrary wave-vector $|\psi\rangle$, which is parallel to the operator.

$$P_{i} | \psi \rangle = | \psi_{i} \rangle \langle \psi_{i} | \psi \rangle$$

$$= \sum_{j=1}^{\infty} C_{j} | \psi_{i} \rangle \langle \psi_{i} | \psi_{i} \rangle = \sum_{j=1}^{\infty} C_{j} | \psi_{i} \rangle \delta_{ij} = C_{i} | \psi_{i} \rangle.$$

Thus we see that all of our old expressions can equivalently be represented in terms of Dirac's "bra" and "ket" notations.

3.4. MATRIX REPRESENTATION OF LINEAR OPERATORS:

Let us consider a complete set of orthonormal functions ψ_i , so that every function ψ can be represented as

$$\psi = \sum_{j} C_{j} \psi_{j}. \qquad \dots (16)$$

Now, let us suppose that the operation of any linear operator 'A' transforms ψ_j into ϕ_j ,

$$i.e., \qquad A\psi_i = \phi_i. \qquad \dots (17)$$

Since ψ_i forms a complete set, we can represent ϕ_i as a linear combination of ψ_i 's as

$$\phi_j = \sum_i a_{ij} \psi_i \qquad \dots (18)$$

or

...

$$A\psi_{j} = \sum_{i} a_{ij} \psi_{i}. \qquad \dots (19)$$

Thus, by knowing the values of a_{ij} for all values of i and j, we can represent the effect of operator 'A' on any function ψ as

$$A\psi = \sum_{j} C_{j} A\psi_{j} = \sum_{i} \sum_{i} C_{j} a_{ij} \psi_{i}. \qquad ...(20)$$

To obtain the numbers a_{ij} , we multiply (19) from left by ψ_i^* and integrate.

$$\int \psi_{i}^{*} A \psi_{j} d^{3}r = \sum_{i} a_{i}^{j} \int \psi_{i}^{*} \psi_{i} d^{3}r = \sum_{i} a_{i}^{j} \delta_{i,j} = a_{i,j},$$

$$\therefore a_{i,j} = \int \psi_{i}^{*} A \psi_{j} d^{3}r \equiv (\psi_{i}, A \psi_{j}) \equiv \langle \psi_{i} \mid A \mid \psi_{j} \rangle \qquad \dots (21)$$

The numbers a_{ij} can be written schematically in a square arrays—

It is the matrix representation of the operator A. The numbers a_{ij} are called matrix elements of A, which is called the matrix A. The subscript i denotes the row and j denotes the column of an element a_{ij} .

3.5. ALGEBRA AND PROPERTIES OF MATRICES:

A matrix with n rows and m columns is called an 'n by m' matrix. If the number of rows is equal to the number of columns, then the matrix is called a Square Matrix.

A matrix, $\begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_n \end{pmatrix}$

composed of only one column is called a column matrix or a column vector. Similarly, a matrix with only one row

$$(C_1, C_2 \ldots C_n)$$

is called a row matrix or row vector. It has been seen that a wavefunction of some physical state can be represented by column vector in the Hilbert space.

A matrix in which all the elements are zero is called a Zero or Null matrix. We shall denote the null matrix of order m by n as $O_{m \times n}$;

$$e.g., O_{2\times 3} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The diagonal going from the top left corner to the bottom right corner of a square matrix is known as the principal diagonal. For a square matrix of order n it is consisted of the element $a_{11}, a_{22}, \ldots a_{nn}$. A square matrix having non vanishing elements only along the principal diagonal is called a Diagonal matrix. It will be of the form:

$$A = \begin{bmatrix} a_{11} & 0 & 0 & \dots & 0 \\ 0 & a_{22} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & a_{nn} \end{bmatrix} \qquad \dots (23)$$

If all the diagonal elements of a diagonal matrix are equal to some constant number C, it is called a *Scalar or constant matrix*. The special case of a constant matrix where C=1 is important, and is called the *Identity or Unit matrix*. We shall denote a unit matrix of order n by I_n , Thus,

$$I_{4} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad \dots (24)$$

If the elements a_{ij} of a matrix A are from the system of complex numbers, we define the conjugate of A by taking the complex conjugate a_{ij}^* of each element a_{ij} and denote it by A^* . If $A^* = A$ for some matrix A, we shall call that as a Real Matrix.

The matrix obtained by interchanging the rows and columns of a matrix A is called its *Transpose* and we shall denote it by A or A. If A = A for some matrix A, it will be called as a *Symmetric matrix*. On the other hand, if A = -A, it will be called an *Antisymmetric or Skew-symmetric matrix*.

If A is a matrix over the complex numbers, then the transpose of its conjugate will be known as *Hermitian Conjugate*. We shall denote it by A^{\dagger} ;

$$A\dagger = (\overrightarrow{A}^*) = (\overrightarrow{A})^*$$

If $A\dagger = A$ for any matrix A, it will be known as a Hermitian matrix. On the other hand, if $A\dagger = -A$, it will be called an Antihermitian or Skew-hermitian matrix.

Addition and Subtraction of Matrices:

The sum of two 'm by n' matrices A and B with respective elements a_{ij} and b_{ij} is defined by the 'm by n' matrix C with elements

$$c_{ij} = a_{ij} + b_{ij} \qquad \dots (25)$$

$$C = A + B$$

and

e.g., if we take

$$A = \begin{bmatrix} 0 & 2 & 0 \\ 1 & 1 & 3 \end{bmatrix} \text{ and } B = \begin{bmatrix} 1 & 0 & 1 \\ 3 & 2 & 4 \end{bmatrix},$$

with

then,
$$C = A + B = \begin{bmatrix} 0+1 & 2+0 & 0+1 \\ 1+3 & 1+2 & 3+4 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1 \\ 4 & 3 & 7 \end{bmatrix}$$

Addition is only defined for matrices that have the same number of rows and the same number of columns.

Subtraction is the reverse of addition and the matrix,

$$D = A - B,$$

 $d_{ij} = a_{ij} - b_{ij}$...(26)

is called the difference of A and B.

From the definition (25) it is obvious that the addition of matrices is both commutative and associative,

i.e.,
$$A+B=B+A$$
 ...(27)

and
$$(A+B)+C=A+(B+C)$$
 ...(28)

Scalar Multiplication and Matrix Multiplication

The product of the matrix A and the constant c is defined to be the matrix cA with elements,

$$(cA)_{ij} = ca_{ij} \qquad \dots (29)$$

The product C=AB of the matrices A and B is defined only when the number of columns of A is equal to the number of rows of B. The elements of the product matrix are given by,

$$C_{ij} = \sum_{k} a_{ik} b_{kj} \qquad ...(30)$$

e.g., if we take

$$A = \begin{bmatrix} 2 & 3 \\ -1 & 2 \\ 0 & 1 \end{bmatrix} \text{ and } B = \begin{bmatrix} 1 & 2 \\ -1 & 4 \end{bmatrix},$$
then, $C = AB = \begin{bmatrix} 2.1 + 3. -1 & 2.2 + 3.4 \\ -1 & 1 + 2. -1 & -1.2 + 2.4 \\ 0.1 + 1. -1 & 0.2 + 1.4 \end{bmatrix} = \begin{bmatrix} -1 & 16 \\ -3 & 6 \\ -1 & 4 \end{bmatrix}.$

Observe that the number of rows of C is equal to the number of rows of A and the number of columns of A is equal to the number of columns of B. Matrix multiplication is not commutative, i.e., in general

$$AB \neq BA$$
 ...(31)

However, matrix multiplication is associative,

i.e.,
$$(AB) C = A (BC)$$
. ...(32)

Also, multiplication is distributive over addition,

If the product of two matrices is a null matrix, then it is not necessary that at least one of them should be a null matrix

i.e,
$$AB=0 \neq A=0 \text{ or } B=0,$$

e.g., $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$

Determinant and Adjoint of a Matrix. If A is a square matrix of order n, we denote its determinant by det (A) or det A or |A|; it is an entity of the same kind as the elements of A.

The determinant of the square matrix of order (n-1), obtained from A by deleting its *i*th row and *j*th column is called the minor of the element a_{ij} . The cofactor of a_{ij} , denoted by A_{ij} , is defined as $(-1)^{i+j}$ times the minor of a_{ij} . The determinant of A, then equals

$$\det A = \sum_{k=1}^{n} a_{ik} A_{ik}, \det A = \sum_{j=1}^{n} a_{ji} A_{ji}, 1 \leqslant i \leqslant n. \qquad ...(34)$$

i.e., the determinant can be expanded in terms of any row or any column of the matrix.

If the determinant of a matrix zero, it is called as a Singular Matrix otherwise it is a non-singular matrix.

To get the adjoint of a matrix, replace each element of the matrix by its cofactor and get the matrix of cofactors:

$$A_{c} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{bmatrix}.$$

Then the transpose of A_c will give the adjoint of the matrix A; i.e.,

$$Adj. A = \overrightarrow{A_c} = \begin{bmatrix} A_{11} & A_{21} & \dots & A_{n_1} \\ A_{12} & A_{22} & \dots & A_{n_2} \\ \vdots & \vdots & \vdots & \vdots \\ A_{1n} & A_{2n} & \dots & A_{nn} \end{bmatrix} \dots (35)$$

Inverse of a Matrix:

The inverse of the square matrix A is the matrix A^{-1} such that $AA^{-1}=A^{-1}A=I$. (36)

This inverse exists if and only if the matrix A is non-singular and it is obtained by dividing the adjoint of A by the (det. A),

and it is obtained by
$$A = \begin{bmatrix} 1 & 0 \\ 2 & 2 \end{bmatrix}$$
, $A = \begin{bmatrix} 1 & 0 \\ 2 & 2 \end{bmatrix}$, then $A^{-1} = \frac{1}{2} \begin{bmatrix} 2 & 0 \\ -2 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -1 & \frac{1}{2} \end{bmatrix}$.

The inverse of the inverse of a matrix is the original matrix.

$$(A^{-1})^{-1} = A ...(37)$$

The inverse of a product is one product of the inverses in reverse order;

$$i.e., (AB)^{-1} = B^{-1}A^{-1}. ...(38)$$

Orthogonal Matrix:

A square matrix whose inverse is equal to its transpose is known as an orthogonal matrix. For an orthogonal matrix A, we have

$$\overrightarrow{AA} = \overrightarrow{A}A = I$$
 or $A^{-1} = \overrightarrow{A}$(39)

Unitary Matrix:

If the inverse of a matrix is equal to its Hermitian conjugate, we call it as Unitary. Thus a square matrix A will be Unitary, if

$$AA\dagger = A\dagger A = I$$
 or $A\dagger = A^{-1}$(40)

Trace of a Matrix:

Trace (or spur) of a matrix is defined as the sum of its diagonal elements;

$$i.e., T_r.A = \Sigma a_{ij},$$

Some Important Identities:

Following identities can easily be verified for the matrices A and B:

$$(AB) = BA,$$
 ...(41)
 $(AB)^* = A^*B^*,$...(42)
 $(AB)^{\dagger} = B^{\dagger}A^{\dagger},$...(43)
 $\det (AB) = (\det A) \cdot (\det B),$...(44)
 $\det A = \det A,$...(45)
 $\det A^* = (\det A)^*$...(46)
 $\det A^{\dagger} = (\det A)^*,$...(47)
 $T_r \cdot (AB) = T_r \cdot (BA)$; ...(48)

3.6. EIGEN-VALUES AND EIGEN-VECTORS OF THE MATRIX OF AN OPERATOR:

We can find the eigenvalues and the eigenvectors of a linear operator if we are given the matrix representation for that operator. In order to find the eigenvalues of an operator A from its matrix representation, we start with the eigenvalue equation,

$$A\psi = \lambda \psi$$
.

Now expanding ψ in a complete orthogonal set, $\psi = \sum_{j} C_{j} \psi_{j}$,

we can write

$$\sum_{i} C_{i} A \psi_{i} = \lambda \sum_{i} C_{i} \psi_{i}.$$

Multiplying this equation from left by ψ_i^* and integrating over the space, we obtain

$$\sum_{j} C_{j} \int \psi_{i} A\psi_{j} d^{3}r = \lambda \sum_{j} C_{j} \int \psi_{i} \psi_{j} d^{3}r$$

$$\sum_{j} C_{j} a_{ij} = \lambda \sum_{j} C_{j} \delta_{ij}.$$

or

In an n-dimensional vector space, it is a set of n equations

$$a_{11}C_{1} + a_{12}C_{2} + \dots + a_{1n}C_{n} = \lambda C_{1}$$

$$\vdots$$

$$a_{n1}C_{1} + a_{n2}C_{2} + \dots + a_{nn}C_{n} = \lambda C_{n},$$

$$i.e., \qquad (a_{11} - \lambda) C_{1} + a_{12}C_{2} + \dots + a_{1n}C_{n} = 0$$

$$\vdots$$

$$a_{n1}C_{1} + a_{n2}C_{2} + \dots + (a_{nn} - \lambda) C_{n} = 0.$$

$$(49)$$

This system of *n*-homogeneous linear equations in the unknowns C_i (i=1, 2, ..., n) has a non-zero solution if and only if the determinant of the matrix of the coefficients is zero; i.e., if

$$\begin{vmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{nn} - \lambda \end{vmatrix} = \det(A - \lambda I) = 0. \dots (50)$$

This determinant, when evaluated, gives a polynomial of degree n in λ , called the characteristic polynomial of A. The roots of this polynomial are the eigenvalues of the operator A. For every eigenvalue, the equations (49) have a solution giving the corresponding eigenvector,

$$\psi = \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_n \end{bmatrix} \dots (51)$$

However, it should be noted that each eigenvector can be multiplied by an arbitrary constant and still remains an eigenvector. Consequently, it is always possible to define normalized eigenvector that satisfy

or
$$\int \psi^* \psi \ d^3r = 1$$

$$\int \sum_{i,j} C_i^* C_j \psi_i^* \psi_j \ d^3r = \sum_{i,j} C_i^* C_j \delta_{ij} = \sum_{i} C_i^* C_i = 1.$$

From it we see that the normalization condition for the eigenvector (51) can be written as

$$\int \psi^* \psi \ d^3r = \langle \psi \mid \psi \rangle = [C_1^* \ C_2^* \dots C_n^*] \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_n \end{bmatrix} = 1. \qquad \dots (52)$$

Thus, if the ket-vector for some system is given by, (51), then the corresponding bra-vector will be written as

$$\langle \psi \mid = [C_1^* \ C_2^* \ \dots \ C_n^*].$$
 ...(53)

As an illustration, let us consider the two by two matrix,

$$A = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

To obtain its eigenvalues and eigenvectors, we write

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \lambda \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}$$

where λ is the eigenvalue and $\begin{bmatrix} C_1 \\ C_2 \end{bmatrix}$ the eigenvector of A.

The eigenvectors of A are the solutions of the simultaneous equations,

$$\begin{array}{c} (1-\lambda) \ C_1 = 0 \\ \text{and} \ (-1-\lambda) \ C_2 = 0 \end{array}$$

These equations have a non-zero solution only when,

$$\begin{vmatrix} (1-\lambda) & 0 \\ 0 & (-1-\lambda) \end{vmatrix} = \lambda^2 - 1 = 0; i.e., \text{ when } \lambda = \pm 1.$$

The corresponding normalized eigenvectors are,

$$\alpha = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
 for $\lambda = 1$; $\beta = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ for $\lambda = -1$.

3.7 CHANGE OF BASIS FUNCTIONS; UNITARY AND SIMILARITY TRANSFORMATIONS:

We may think of more than one complete set of orthonormal basis functions in a Hilbert space. Correspondingly, there will be a different matrix for an operator w.r.t. these basis. New we shall see that how to find the matrix of an operator in any representation from some other representation. For it let us consider two different complete set of orthonormal functions, viz. ψ_i and ϕ_i , which span the same Hilbert space. An arbiratry wavefunction ψ can be expanded in terms of these complete set of functions as:

$$\psi = \sum_{j} C_{j} \psi_{j} = \sum_{i} f_{i} \phi_{i} \qquad ...(54)$$

Also the members '\phi' of the other set can be expanded in terms of ψ_i as

 $\phi_i = \Sigma u_{pi} \psi_p$; i=1, 2, 3,(55)

where u_{pi} are the expansion coefficients and form an infinite matrix U.

Similarly,

$$\psi_i = \sum_{q} v_{qi} \phi_q; i=1, 2, 3,...$$
 ...(56)

where v_{ql} form an infinite matrix V.

Substituting (56) into (55), we get

$$\phi_{i} = \sum_{p} u_{pi} \sum_{q} v_{qp} \phi_{q} = \sum_{q} (\sum_{p} v_{qp} u_{pi}) \phi_{q}$$

$$\Rightarrow \sum_{p} v_{qp} u_{pi} = \delta_{qi}$$

In matrix language it reads as

$$VU=I$$
 ...(57)

Similarly, substituting (55), into (56), we get UV = I

From (57) and (58) we have

$$V = U^{-1}$$
 or $V^{-1} = U$

Hence we see that if we can transform from the representation ψ_i to ϕ_i with the application of the matrix U we can get the reverse with the matrix U^{-1} . Here U is called as the Transformation Matrix. A transformation from one representation to another is analogous to the rotation of coordinate axes in 3-d cartesian space.

As both basis sets are orthonormal, we have

$$\delta_{ij} = \int \phi_i^* \phi_j \ d^3r = \int \sum_{\substack{p \ q \ p}} \sum_{\substack{q \ p}} u_{pi}^* \psi_p^* . u_{qj} \psi_q \ d^3r$$

$$= \sum_{\substack{p, \ q \ p}} u_{pi}^* u_{qj} \ \delta_{pq} = \sum_{\substack{p \ q \ p}} u_{pi}^* u_{pj}$$

$$= \sum_{\substack{p \ q \ p}} (U^*)_{ip} (U)_{pj}$$

$$= \sum_{\substack{p \ q \ p}} (U^{\dagger})_{ip} (U)_{pj} \{(U)_{ij} \text{ is the } i\text{-}j \text{ th element of } U\}.$$

In matrix notation it can be written as

 $U\dagger U=I \text{ or } U\dagger =U^{-1},$

i.e., the matrix transforming one orthonormal set into another is unitary and hence the transformation of this type is termed as Unitary transformation.

Now we find the relation between the coefficients C_i and f_i of expansions (54). For it we write,

nsions (54). For it we write,

$$\psi = \sum_{i} f_{i} \phi_{i} = \sum_{i} f_{i} \sum_{p} u_{pl} \psi_{p} = \sum_{p} (\sum_{i} u_{pi} f_{i}) \psi_{p}.$$

Also,
$$\psi = \sum_{p}^{i} C_{p} \psi_{p}.$$

Commparing these,

$$C_p = \sum_{i} u_{pi} f_i$$
 or $C_j = \sum_{i} u_{ji} f_i$; $j = 1, 2,$ (61)

i.e. C=UF ...(62)

$$C = \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_j \end{bmatrix} \text{ and } F = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_i \end{bmatrix}$$

Hence we can find the wavefunction in the transformed representation, if we know it in the original representation, with the help of the transformation matrix.

To close the section, we find the relation between the matrix representations of a linear operator w.r.t. two different basis connected by a unitary transformation. Let us represent by $A^{(1)}$ and $A^{(2)}$, the matrices of a linear operator 'A' w.r.t. the basis functions ψ_i and ϕ_i , respectively.

Whe have

$$a_{ij}^{(1)} = \int \psi_{i}^{*} A \psi_{j} d^{3}r ; a_{ij}^{(2)} = \int \phi_{i}^{*} A \phi_{j} d^{3}r \qquad ...(63)$$
Using (55) we have
$$a_{ij}^{(2)} = \int \sum_{p} u_{pi}^{*} \psi_{p}^{*} A \sum_{q} u_{qj} \psi_{q} d^{3}r \qquad ...(63)$$

$$= \sum_{p,q} u_{pi}^{*} \left(\int \psi_{p}^{*} A \psi_{q} d^{3}r \right) u_{qj}$$

$$= \sum_{p,q} u_{pi}^{*} a^{(1)}_{pq} u_{qj}$$

$$= \sum_{p,q} (U^{*})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{*})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

$$= \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{piq} (U)_{qj} = \sum_{p,q} (U^{\dagger})_{ip} a^{(1)}_{pq} U_{qj}$$

This type of transformation of the matrix $A^{(1)}$ into $A^{(2)}$ is known as the similarity transformation. Thus the relation between the matrix $A^{(1)}$ and the transformed matrix $A^{(2)}$ is a Similarity transformation by the transformation matrix U.

3.8. PROPERTIES OF UNITARY TRANSFORMATION

Following are the important properties of a unitary transformation.

(I) The normalization of an arbitrary function is left unchanged. To prove it, let us represent an arbitrary function ψ in two representations ϕ_i and ϕ_i as:

$$\psi = \sum_{i} C_{i} \psi_{i}$$
 and $\psi = \sum_{i} f_{i} \phi_{i}$...(65)

Then we have

$$C_j = \sum_{i} u_{ji} f_i, \quad j = 1, 2, \dots$$
 ...(66)

If ψ is normalized in the ψ_t representation, then

$$\sum_{j} C_{j} * C_{j} = 1 \qquad \dots (67)$$

Now

$$\Sigma C_{j} * C_{j} = \Sigma \Sigma \Sigma u_{ji} * u_{ji} f_{i} * f_{i}$$

$$= \Sigma \Sigma \Sigma (U\dagger)_{ij} (U)_{ji} f_{i} * f_{i}$$

$$= \Sigma \Sigma \delta_{ji} f_{i} * f_{i} = \Sigma f_{i} * f_{i}$$
...(68)

From (68) and (67), we see that $\sum_{i=1}^{n} f_i = 1$;

i.e., the function ψ is normalized in the ϕ_l representation. Hence the normalization of an arbitrary function is left unchanged.

(II) The orthogonal functions are transformed into functions which remain orthogonal. To prove this property, we consider the following integral, which is zero for two orthogonal functions ψ and ϕ :

$$\int \psi^* \, \phi \, d^3r = \int \phi^* \, \psi \, d^3r = 0$$

If ψ and ϕ are expanded in series of ψ_i , we get $\psi = \sum_j C_j \psi_j$ and $\phi = \sum_j C'_j \psi_j'$

and

$$\int \psi^* \phi \ d^3r = \int \sum_{jj'} C_{j}^* C_{j}^* C_{j}' \psi_{j}^* \psi_{j}' \ d^3r = \sum_{jj'} C_{j}^* C_{j}' \delta_{jj}'$$

$$= \sum_{j} C_{j}^* C_{j}'$$

Under a unitary transformation we have $C_i = \sum_i u_{ii} f_i$

$$C_{j}^{*} = \sum_{i} u_{ji}^{*} f_{i}^{*} = \sum_{i} (U_{1}^{i})_{ij} f_{i}^{*}$$

$$C_{j}' = \sum_{i} u_{ji} \cdot f_{i}' = \sum_{i} (U)_{ji} f_{i}'$$

where f_i and f_i are the coefficients of expansion for ϕ and ψ ; respectively, in series of ϕ_i .

Now

$$\int \psi^* \phi \ d^3r = \sum_j C_j^* C_j' = \sum_j \sum_i (U\dagger)_{ij} (U)_{ji} f_i^* f_i'$$

$$= \sum_i \sum_i \delta_{ii} f_i^* f_i' = \sum_j f_i^* f_i'$$

We conclude that the expansion of $|\psi^* \phi d^3r|$ takes the same form in all representations, so that if it is zero in any one representation, it is also zero after a unitary transformation has been carried out. Thus, the orthogonality properties of a set of wavefunctions are left unchanged by a unitary transformation.

Relationship between transformed operators remains the same as those between the corresponding untransformed operators.

Consider for example a matrix equation.

$$A^{(1)}B^{(1)} = C^{(1)}D^{(1)}E^{(1)} + F^{(1)};$$

in the first representation. In order to find this equation in the second representation we apply the similarity transformation of equation (64). We get

or
$$U^{-1}A^{(1)}B^{(1)}U = U^{-1}C^{(1)}D^{(1)}E^{(1)}U + U^{-1}F^{(1)}U$$

or $U^{-1}A^{(1)}U.U \quad {}^{1}B^{(1)}U = U^{-1}C^{(1)}U \quad {}^{U^{-1}D^{(1)}}UU^{-1}E^{(1)}U + U^{-1}F^{(1)}U$
or $A^{(2)}B^{(2)} = C^{(2)}D^{(2)}E^{(2)} + F^{(2)}$

Similarly we can prove for any other relationship of the operators, that the form of the relationship remains unaltered under a unitary transformation.

(IV) The eigenvalues of a matrix are not changed by a unitary transformation.

Suppose the operator A is represented by the matrix $A^{(1)}$ in the original representation. The eigenvalue & satisfies

$$A^{(1)}C=\lambda C$$

where C is the representative of the eigenfunction. If the basis functions ase transformed, the operator matrix undergoes a similarity transformation

$$A^{(1)} = UA^{(2)}U^{-1}$$

and the eigenvalue equation may be written as

$$UA^{(2)}U^{-1}C=\lambda C.$$

On premultiplying by U^{-1}

$$A^{(2)}(U^{-1}C) = \lambda (U^{-1}C).$$

From (62) this becomes

$$A^{(2)}F = \lambda F,$$

where F is the eigenfunction representative in the new basis and hence we see that the eigenvalues of a matrix do not change.

Remarks. Thus we see that from a given representation, we can, by means of a unitary transformation, obtain and equivalent representation of all the quantum mechanical relationship. It is often convenient to transform from one representation into ano3

ther in this way, because it usually turns out that each problem has some representation in which it is most simply expressed. In the classical limit, a unitary transformation of a function produces a canonical transformation of the classical momentum and position coordinates. Thus a unitary transformation is the quantum generalization of the classical concept of a canonical transformation. For this reason a unitary transformation is sometimes also called a canonical transformation.

3.9. CONCEPT OF CONTINUOUS MATRICES:

So far we have considered the expansion of an arbitrary wavefunction in terms of only a discrete set of functions and have thus obtained discrete matrices. If some operator has a continuous set of orthonormal eigenfunctions, we shall obtain a continuous matrix for that. As an example, $\psi(\mathbf{r}, t)$ can be expanded in terms of the momentum eigenfunctions by the Fourier integral as

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi(\mathbf{p}, t) e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} d^3 p, \qquad ... (69)$$

where the orthonormal functions are now the continuous set of momentum eigenfunctions, $\frac{1}{(2\pi\hbar)^{3/2}}e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$, and $\phi(\mathbf{p}, t)$ are the corresponding expansion coefficients.

A matrix element can than be written in analogy with equation (21),

$$a_{pp'} = \frac{1}{(2\pi\hbar)^3} \int e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} A e^{i\mathbf{p} \cdot \mathbf{r}} d^3r, \dots (70)$$

app' is continuous function of p and p', but it may be regarded as the limit of a discrete square array in which the elements are allowed to approach closer and closer to each other. Continuous matrices may be treated in essentially the same way as the discrete matrices. From the equation,

$$\frac{1}{(2\pi\hbar)^3} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \cdot e^{i\mathbf{p}'\cdot\mathbf{r}/\hbar} d^3r = \delta (\mathbf{p} - \mathbf{p}'),$$

we see that the unit matrix becomes the Dirac delta function, $\delta(\mathbf{p}-\mathbf{p}')$. A diagonal mitrax will take the form $C(\mathbf{p})$ $\delta(\mathbf{p}-\mathbf{p}')$. The rule for taking products of continuous matrices reads as

$$(AB)_{\mathbf{p}\mathbf{p}'} = \int A_{\mathbf{p}\mathbf{p}''} B_{\mathbf{p}''\mathbf{p}'} d^3p''. \qquad \dots (71)$$

Samilarly we can define all the other operations for continuous matrices also.

3.10. VARIOUS QUANTUM MECHANICAL PICTURES:

We know that the problems of the classical mechanics can be solved by Newtonian Mechanics or Lagrangian Mechanics or the Hamiltonian Mechanics. All the three types of mechanics adopts quite diffierent formalisms yet they give exactly the same solution of any classical problem, i.e., they are all equivalent. We can thus consider them as three different pictures of the classical mechanics. Similarly, we can have different pictures of the luantum Mechanics, provided that each picture provides an uivalent description of a Quantum Mechanical problem. For it,

(i) The expectation value of an operator should be the same every picture and

(ii) The scalar product of any two states in each picture

ould remain unaltered.

If these two conditions are satisfied, then the eigenvalues and e orthonormality of the quantum mechanical states remain the me and the description of the system is independent of the cture we are using.

Let us consider a picture in which the system under study is presented by the ket $|\psi\rangle$, which is a unit vector in a Hibert pace, in which sets of axes can be defined by the eigenkets of amplete sets of observables of the system. ($|\psi\rangle$ is a unit vector ecause for normalized ψ , its length will be unity). Let in anoner picture the same system be represented by the ket $|\psi'\rangle$, then $|\psi'\rangle$ is given by a unitary transformation of the first picture,

$$|\psi\rangle = U|\psi\rangle, \qquad ...(72)$$

where U is the unitary transformation matrix (operator).

If A is a matrix operator in the first picture, then the corresponding operator A' in the second picture is given by a similarity transformation

$$A' = UAU^{\dagger}$$

Thus, using (72), we can write

$$\langle \psi' \mid A' \mid \psi' \rangle = \langle \psi \mid U \dagger U A U \dagger U \mid \psi \rangle$$

 $=\langle \psi \mid A \mid \psi \rangle \{ U \text{ is unitary} \}.$

Thus the expectation value of an operator in both the pictures is the same. Also we have

$$\langle \psi' \mid \psi' \rangle = \langle \psi \mid U \uparrow U \mid \psi \rangle = \langle \psi \mid \psi \rangle$$
.

Hence the second condition, that the scalar product should remain unaltered, is also satisfied. Thus we conclude that a picture, and the picture obtained by a unitary transformation of it, are equivalent in all respects to describe the dynamics of a system. As there may be an infinite number of unitary transformations performed on a picture, we can have infinite number of pictures corresponding to these However, we shall discuss only three pictures which are used in quantum mechanics.

(I) Schroedinger Picture:

We have seen that in quantum mechanics, a system is represented by a space time wavefunction $\psi(\mathbf{r}, t)$, which obeys the Schroedinger equation

$$i\hbar \frac{d\psi}{dt} = H\psi. \qquad ...(73)$$

Equation (73) has an analogy in matrix theory. Let $\{\psi_t\}$ be a complete set of time-independent orthonormal basis functions which can be used to expand ψ (\mathbf{r} , t) as

$$\psi(\mathbf{r},t) = \sum_{j} C_{j}(t) \psi_{j}(\mathbf{r}). \qquad ...(74)$$

Putting this ψ (r, t) in (73), we get

$$\sum_{j} HC_{j}(t) \psi_{j}(\mathbf{r}) = i \hbar \sum_{j} \frac{dC_{j}(t)}{dt} \psi_{j}(\mathbf{r}).$$

Multiplying this equation from left by ψ_i^* (r) and integrating over all space we get

$$\sum_{j} H_{ij} C_{j}(t) = i\hbar \frac{dC_{i}(t)}{dt},$$

where

$$H_{ij} = \int \psi_i^* H \psi_j d^3r.$$

In terms of matrices

$$H \mid \psi(t) \rangle = i \hbar \frac{d}{dt} \mid \psi(t) \rangle,$$
 ... (75)

where $|\psi(t)\rangle$ is the column vector,

$$| \psi(t) \rangle = \begin{bmatrix} C_1(t) \\ C_2(t) \\ \vdots \\ C_j(t) \end{bmatrix}$$

This representation of the wavefunction is known as the Schroedinger picture. The dynamics of the system in this picture is governed by the Schroedinger equation (75). In this picture, the wavefunctions are time dependent while the operators, which are functions of x and p, are time independent.

The expectation value of any physical observable A at time is given by

 $\langle A \rangle_i = \langle \psi(t) \mid A \mid \psi(t) \rangle.$...(76)

(II) Heisenberg Picture:

In this picture, in contrast to the Schroedinger picture, the operators are time dependent while the wavefunctions are time independent. The dynamics of the system is described by the Heisenberg equation of motion.

$$A_H = \frac{1}{i\hbar} [A_H, H_H].$$
 ...(77)

The subscript H here specifies the Heisenberg picture A_H is any operator and H_H is the Hamiltonian operator in this picture.

To find the unitary transformation which gives this picture from the Schroedinger picture, we require that the two pictures should coincide at t=0. Now, formally integrating the Schroedinger equation (75), we have

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle \equiv e^{-iHt/\hbar} |\psi_H\rangle \qquad ...(78)$$

The value of the Schroedinger wavefunction at time t=0, $\psi(0)$, is the Heisenberg wavefunction ψ_H . Since it is time independent,

$$\frac{d |\psi_H\rangle}{dt} = 0 \qquad \dots (79)$$

From (78), we have

$$|\psi_H\rangle = e^{iHt/\hbar}|\psi(t)\rangle$$
 ...(80)

Thus the transformation matrix $U=e^{iHt/\hbar}$

Since the Hamiltonian H which gives the total energy of a system is Hermitian, because the energy of any system is always real, U must be unitary. Thus eqn. (80) gives the unitary transformation from the Schroedinger picture to the Heisenberg picture.

In order to find the relationship between the time independent operator A of the Schroedinger picture and the time dependent operator A_H of the Heisenberg picture, we note that the expectation value of the operator in the two pictures should be the same

i.e.,
$$\langle \psi | A | \psi(t) \rangle = \langle \psi_H | A_H | \psi_H \rangle$$

or $\langle \psi(t) | A | \psi(t) \rangle = \langle \psi(t) | e^{-iHt/\hbar} A_H e^{iHt/\hbar} | \psi(t) \rangle$
 $\Rightarrow A = e^{-iHt/\hbar} A_H e^{iHt/\hbar}$

or
$$A_H = e^{iHt/\hbar} A e^{-iHt/\hbar}$$
 ...(81)

Hence the Heisenberg's operators are given by a similarity transformation of the Schroedinger's operators.

From (81) we see that

$$H_{H} = e^{iHt/\hbar} H e^{-iHt/\hbar}$$

$$= H e^{iHt/\hbar} e^{-iHt/\hbar} = H;$$

i.e., the Hamiltonian operator does not change with time, even in the Heisenberg picture. It is identical to the Hamiltonian of the Schroedinger picture. Thus, now onwards we shall be omitting the subscript H for Hamiltonian operator.

(III) Interaction Picture:

Lastly we consider a picture which is intermediate between the above two pictures. In this picture the time dependence is carried by both the operators as well as the state-vectors. This is called the interaction picture and to specify it we divide the Hamiltonian into two parts,

$$H_I = H_{0I} + H'_I \qquad \dots (82)$$

is such that H_{of} does not depend on time and also has a simple . 7 ... structure, and H'_I gives some additional interaction and depends explicitly on time. The operators A_I and the state vector $|\psi_I\rangle$ of this picture are related to the Schroedinger picture by the unitary transformation

$$A_{I} = e^{iH_{0}t/\hbar} A e^{-iH_{0}t/\hbar} \qquad ...(83)$$

$$|\psi_l\rangle = e^{iH_0t/\hbar} |\psi(t)\rangle \qquad ...(84)$$
He isophers pictures are the same when

so that the interaction and Heisenberg pictures are the same when $H'_{I}=0$. We have shown that $H_{H}=H$, and eqn. (84) shows that $H_{0I}=H_0$. Differentiation of (84) gives the equation of motion of ψ1>,

$$i\hbar \frac{d}{dt}|\psi_{l}\rangle = -H_{0}e^{iH_{0}t/\hbar}|\psi(t)\rangle + e^{iH_{0}t/\hbar}.i\hbar \frac{d|\psi(t)\rangle}{dt}$$

Now, if
$$\frac{d \mid \psi(t) \rangle}{dt} = H \mid \dot{\psi}(t) \rangle = (H_0 + H') \mid \psi(t) \rangle$$

$$i\hbar \frac{d |\psi_{I}\rangle}{dt} e^{iH_{0}t/\hbar} H' |\psi(t)\rangle$$

$$= e^{iH_{0}t/\hbar} H' e^{-iH_{0}t/\hbar} e^{iH_{0}t/\hbar} |\psi(t)\rangle$$

$$= d |\psi_{I}\rangle \qquad (85)$$

i.e.,
$$i \frac{d |\psi_I\rangle}{dt} = H'_I |\psi_I\rangle \qquad ...(85)$$

To get the equation of motion for the operator A, of this picture, we differentiate (83) w.r.t. time,

$$\frac{dA_I}{dt} = \frac{1}{i\hbar} [A_I, H_{oI}] + \frac{\partial A_I}{\partial t} \qquad ...(86)$$

If A_I does not depend explicitly on time,

$$\frac{dA_I}{dt} = \frac{1}{i\hbar} [A_I, H_{oI}] \qquad ...(87)$$

Equations (85) and (87) describe the dynamics of the system in the interaction picture. It is clear that the state-vectors $|\psi_I(t)\rangle$ satisfy an equation of the form of the Schroedinger picture with the time dependent part of the Hamiltonian, H'_I , and the operators A_I satisfy an equation of the form of Heisenberg picture with the time independent part of the Hamiltonian.

Remarks:

We have seen that the state of a system at any time is described by a unit-vector $|\psi\rangle$, in the Hilbert space. Any change with time in the state of the system can be investigated by keeping the axes fixed and allowing the state vector to rotate, or by keeping the state vector fixed and allowing the axes to rotate, or by permitting simultaneous rotation of the state vector and of the axes. The three possibilities are the Schroedinger, the Heisenberg and the interaction "pictures" respectively.

Table below gives the equations of motion of the state vector $|\psi\rangle$ and of any observable A of the system in each of three pictures. Subscripts H and I denote "Heisenberg" and "interaction" respectively. Quantities without subscripts refer to the Schroedinger picture. Relations between the corresponding entities in the different pictures also given.

Schroedinger picture	$i\hbar \frac{d \psi(t)\rangle}{dt} = H \psi(t)\rangle, \frac{dA}{dt} = 0$
Heisenberg picture	$\begin{vmatrix} \frac{d \mid \psi_{H} \rangle}{dt} = 0, & \frac{d A_{H}}{dt} = \frac{1}{i \hbar} [A_{H}, H_{H}] \\ \psi_{H}\rangle = e^{iHt/\hbar} \psi(t)\rangle, & A_{H} = e^{iHt/\hbar} A e^{-iHt/\hbar} \end{vmatrix}$
Interaction picture	$i\hbar \frac{d \mid \psi_{I}(t) \rangle}{dt} = H'_{I} \mid \psi_{I}(t) \rangle, \frac{d A_{I}}{dt} = \frac{1}{t\hbar} [A_{I}, H_{0I}]$ $\mid \psi_{I} \rangle e^{iH_{0}t/\hbar} \mid \psi(t) \rangle, A_{I} = e^{iH_{0}t/\hbar} A e^{-iH_{0}t/\hbar}$ $H_{I} = H_{0I} + H'_{I}$

3.11. MARIX THEORY OF HARMONIC OSCILLATOR:

The Hamiltonian for the one-dimensional harmonic oscillator is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \qquad ...(88)$$

where the first term gives the kinetic energy and the second term gives the potential energy, x and p are the position and the momentum operators and satisfy the quantum condition.

$$xp-px=i\hbar. ...(89)$$

We define the operators a and at, called the lowering and the raising operators respectively, as

$$a = \frac{1}{\sqrt{(2\hbar m\omega)}} (m\omega x + ip)$$

$$a \dagger = \frac{1}{\sqrt{(2\hbar m\omega)}} (m\omega x - ip).$$

$$(90)$$

Then,

$$a\dagger a = \frac{1}{2\hbar m\omega} \left[m^{2}\omega^{2}x^{2} + im\omega (xp - px) + p^{2} \right]$$

$$= \frac{1}{2\hbar m\omega} \left[m^{2}\omega^{2}x^{2} + im\omega . i\hbar + p^{2} \right]$$

$$= \frac{1}{2\hbar m\omega} \left[p^{2} + m^{2}\omega^{2}x^{2} - \hbar m\omega \right]$$

$$= \frac{1}{\hbar \omega} \left[\frac{p^{2}}{2m} + \frac{1}{2} m\omega^{2}x^{2} \right] - \frac{1}{2}$$

$$= \frac{H}{\hbar \omega} - \frac{1}{2}(91)$$

Similarly,

$$g_{\alpha}^{Q}a\dagger = \frac{H}{\hbar\omega} + \frac{1}{2}.$$
 ...(92)

From (91) and (92), we have

$$aa\dagger - a\dagger a = 1,$$
 ...(93)

i.e., a and $a\dagger$ do not commute with each other and hence we can not measure these simultaneously. On the other hand, it is clear from (91) and (92) that the Hamiltonian commutes with $a\dagger a$ and $aa\dagger$. Thus the eigenvectors of H and $aa\dagger$ or $a\dagger a$ can be assumed to be the same. Hence, it is sufficient to solve the eigenvalue problem for $a\dagger a$ or $aa\dagger$. Representing the eigenvalues by, λ_k , and the corresponding eigenvectors by, $|k\rangle$, we can write the eigenvalue equation for $a\dagger a$ as

$$a \dagger a \mid k \rangle = \lambda_k \mid k \rangle$$
.

To solve this equation for λ_k , we first find out $a \uparrow | k \rangle$ and $a \mid k$). For it, we have from (93),

or
$$a\dagger aa\dagger - a\dagger a = a\dagger$$

$$(a\dagger a) \ a\dagger = a\dagger \ (a\dagger a + 1).$$

$$(a\dagger a) \ a\dagger \ | \ k\rangle = a\dagger \ (a\dagger a + 1) \ | \ k\rangle$$

$$= a\dagger \ (\lambda_k + 1) \ | \ k\rangle$$

$$= (\lambda_k + 1) \ a\dagger \ | \ k\rangle.$$

Equation (95) tells us that a + k is also an eigenvector of $a\dagger a$ with eigenvalue (λ_k+1) ,

i.e.,
$$a\dagger | k \rangle = C | (k+1) \rangle$$
,

where C is some constant. We choose it so that the eigenvector is normalized,

or
$$|C|^{2} \langle (k+1) \mid (k+1) \rangle = \langle k \mid aa\dagger \mid k \rangle$$
or
$$|C|^{2} = \langle k \mid a\dagger a+1 \mid k \rangle$$
or
$$|C|^{2} = (\lambda_{k}+1).$$

$$: C = \sqrt{(\lambda_{k}+1)} e^{i\alpha},$$

where $e^{i\alpha}$ is an arbitrary phase factor.

$$\therefore a\dagger |k\rangle = \sqrt{(\lambda_k + 1)} e^{i\alpha} |k+1\rangle. \qquad ...(96)$$

In an exactly similar manner, we get

$$a \mid k \rangle = \sqrt{(\lambda_k)} e^{i\alpha} \mid k-1 \rangle.$$
 ...(97)

From (96) and (97), we see that the operation of 'a†' on $|k\rangle$ creates one more state and hence acts as raising operator. On the other hand 'a' destroys one state and hence acts as a lowering operator. ata, preserves the number of states.

We are now ready to find out the possible values of λ_k . have

 $\langle k \mid a \dagger a \mid k \rangle = \lambda_k \langle k \mid k \rangle \geqslant 0$ {: $\langle k \mid a \dagger a \mid k \rangle$ is the norm of the state $a \mid k \rangle$ and therefore it is positive definite}

$$\Rightarrow \lambda_k \geqslant 0$$
 {: $\langle k \mid k \rangle$ is the norm of $\mid k \rangle$ and hence it is + ive}.

Now, applying the lowering operator repeatedly, we can generate, from any given eigenvector, $|k\rangle$, new eigenvectors with different eigenvalues. However, condition $\lambda_k \geqslant 0$ limits the number of times a lowering operator can be applied. When by successive downwards steps an eigenvalue between 0 and 1 is reached, by applying a once more, we do not obtain a new eigenvector, because that will be an eigenvector violating the restriction, $\lambda_k \ge 0$.

Hence, we must have for lowest step (labelled k=0),

 $a\dagger a \mid 0\rangle = \lambda_0 \mid 0\rangle$; $1 \triangleright \lambda_0 \geqslant 0$

and

 $a \mid 0 \rangle = 0 \mid 0 \rangle$.

Consequently, $\lambda_0 = 0$, and this is the only eigenvalue below unity.

Starting from $| 0 \rangle$ and $\lambda_0 = 0$, we obtain all other eigenvectors and eigenvalues by repeated application of the raising operator, at. The eigenvalues increase in unit steps. Thus

 $|k\rangle \propto (a\dagger)^k |0\rangle; k=0, 1, 2, ...$.(98)and

To find the eigenvalues of the Hamiltonian 'H' for the harmonic oscillator, we have from (91),

$$E_k \mid k \rangle = H \mid k \rangle = \hbar \omega \, (a \dagger a + \frac{1}{2}) \mid k \rangle = \hbar \omega \, (k + \frac{1}{2}) \mid k \rangle.$$

 $\vdots \quad E_k = \hbar \omega \, (k + \frac{1}{2}) \; ; \; k = 0, 1, 2, \dots$...(99)

It will be seen in chapter 6 that this is exactly the same as we get in the wave-mechanical treatment by solving the Schroedinger equation for Harmonic Oscillator. For the wave functions of the oscillater see problem 36 of this chapter.

PROBLEMS

Examine the linear independence or dependence of Problem 1. the system of vectors: (2, -1, 3) (0, 1, -2) (8, 2, 0).

Sol. Let
$$u_1 = (2, -1, 3),$$

 $u_2 = (0, 1, -2),$
 $u_3 = (8, 2, 0).$

and

Now, if

$$\alpha_1 u_1 + \alpha_2 u_2 + \alpha_3 u_3 = 0$$
,

then we should have

or
$$\alpha_{1}(2, -1, 3) + \alpha_{2}(0, 1, -2) + \alpha_{3}(8, 2, 0) = (0, 0, 0)$$

$$(2\alpha_{1} + 8\alpha_{3}, -\alpha_{1} + \alpha_{2} + 2\alpha_{3}, 3\alpha_{1} - 2\alpha_{2}) = (0, 0, 0)$$

$$\Rightarrow 2\alpha_{1} + 8\alpha_{3} = 0.$$

$$-\alpha_{1} + \alpha_{2} + 2\alpha_{3} = 0$$
and
$$3\alpha_{1} - 2\alpha_{2} = 0.$$

and

Solving these equations for α_1 , α_2 and α_3 , we get

$$\frac{\alpha_1}{2} = \frac{\alpha_2}{3} = -2\alpha_3 = \lambda,$$

where λ is an arbitrary number. In particular $\alpha_1=2$, $\alpha_2=3$ and $\alpha_3 = -\frac{1}{2}$ is a solution. Thus u_1 , u_2 , u_3 are linearly dependent.

Problem 2. In the following case, find the value of x for which the given set of vectors is linearly dependent: (1, 2, 3), (4, 5, 6) and (x, 8, 9).

Sol. Let
$$u_1 = (1, 2, 3),$$
 $u_2 = (4, 5, 6)$
and $u_3 = (x, 8, 9).$
Now $\alpha_1 u_1 + \alpha_2 u_2 + \alpha_3 u_3 = 0$...(1)
 $\Rightarrow \alpha_1 (1, 2, 3) + \alpha_2 (4, 5, 6) + \alpha_3 (x, 8, 9) = (0, 0, 0)$
or $(\alpha_1 + 4\alpha_2 + x\alpha_3, 2\alpha_1 + 5\alpha_2 + 8\alpha_3, 3\alpha_1 + 6\alpha_2 + 9\alpha_3) = (0, 0, 0)$
or $\alpha_1 + 4\alpha_2 + x\alpha_3 = 0,$...(ii)
 $2\alpha_1 + 5\alpha_2 + 8\alpha_3 = 0$
and $3\alpha_1 + 6\alpha_2 + 9\alpha_3 = 0.$

For the given set to be linearly dependent, equation (i) should be satisfied without all the α_1 , α_2 , α_3 being zero simultaneously, i.e. the equation (ii) should have a non-zero solution, for which the determinant of the matrix of coefficients should be zero

$$\begin{vmatrix} 1 & 4 & x \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{vmatrix} = 0 \Rightarrow x = 7 \text{ on evaluation.}$$

Problem 3. Obtain a set of four orthonormal vectors from the vectors:

ors:

$$u_1=(1, 1, 0, 1), \quad u_2=(2, 0, 0, 1), \quad u_3=(0, 2, 3, -2) \text{ and}$$

 $u_4=(1, 1, 1, -5).$

Sol. We shall do it by Schmidt's method.

Let $v_1 = u_1 = (1, 1, 0, 1)$.

Then $v_2 = u_2 + a_{21}v_1$,

where

$$a_{21} = -\frac{(v_1, u_2)}{(v_1, v_1)} = -\frac{(1.2 + 1.0 + 0.0 + 1.1)}{(1.1 + 1.1 + 0.0 + 1.1)} = -\frac{3}{3} = -1.$$

$$\therefore v_2 = u_2 - v_1 = (2, 0, 0, 1) - (1, 1, 0, 1) = (1, -1, 0, 0).$$

Now take $v_8 = u_3 + a_{31}v_1 + a_{32}v_2$; where

$$a_{31} = -\frac{(v_1, u_3)}{(v_1, v_1)} = 0$$
 and $a_{32} = -\frac{(v_2, u_3)}{(v_2, v_2)} = 1$ on evaluation.
 $v_3 = u_3 + v_2 = (1, 1, 3, -2).$

Finally we take $v_4 = u_4 + a_{41}v_1 + a_{42}v_2 + a_{43}v_3$, where

$$a_{41} = -\frac{(v_1, u_4)}{(v_1, v_1)} = 1.$$

$$a_{42} = -\frac{(v_2, u_4)}{(v_2, v_2)} = 0,$$

$$a_{43} = -\frac{(v_3, u_4)}{(v_3, v_3)} = -1.$$

$$= u_2 + v_1 - v_2 = (1, 1, -2, -2)$$

$$v_4 = u_2 + v_1 - v_3 = (1, 1, -2, -2).$$

The vectors v_1 , v_2 , v_3 , v_4 are orthogonal to each other. In order to find the orthonormal set, we divide each of these by its norm, we get

$$w_1 = \frac{1}{\sqrt{(3)}} (1, 1, 0, 1);$$
 $w_2 = \frac{1}{\sqrt{(2)}} (1, -1, 0, 0);$ $w_3 = \frac{1}{\sqrt{(15)}} (1, 1, 3, 2) \text{ and } w_4 = \frac{1}{\sqrt{(10)}} (1, 1, -2, -2).$

Problem 4. Prove the following properties of the projection operator P_i .

(i) $P_i^2 = P_i$,

Sol. (i)
$$P_i^2 \mid \psi \rangle = P_i \left[P_i \mid \psi \rangle \right]$$

 $= P_i \mid \psi_i \rangle \langle \psi_i \mid \psi \rangle$
 $= \mid \psi_i \rangle \langle \psi_i \mid \psi_i \rangle \langle \psi_i \mid \psi \rangle$
 $= \mid \psi_i \rangle \langle \psi_i \mid \psi \rangle \quad \{ \because \langle \psi_i \mid \psi_i \rangle = 1 \}$
 $= P_i \mid \psi \rangle \Rightarrow P_i^2 = P_i$.

(ii)
$$P_i P_j = | \psi_i \rangle \langle \psi_i | \psi_j \rangle \langle \psi_j |$$

 $= | \psi_i \rangle \langle \psi_j | \delta_{ij} \quad \{ \Upsilon \quad \langle \psi_i | \psi_j \rangle = \delta_{ij} \}$
 $= | \psi_i \rangle \langle \psi_i | \delta_{ij} \quad \text{or} \quad | \psi_j \rangle \langle \psi_j | \delta_{ij}$
 $= P_i \delta_{ij} \quad \text{or} \quad P_j \delta_{ij}.$

Problem 5. Show that

$$\langle n \mid m \rangle = \Sigma \langle n \mid i \rangle \langle i \mid m \rangle$$

where $|n\rangle$ and $|m\rangle$ are two arbitrary vectors and the vectors $|i\rangle$ form a complete set.

Sol. Since the vectors $|i\rangle$ form a complete set, we can write the arbitrary vectors $|n\rangle$ and $|m\rangle$ as

$$|n\rangle = \sum_{i} c_{i} |i\rangle, c_{i} = \langle i | n\rangle,$$

$$|m\rangle = \sum_{i} d_{i} |i\rangle, d_{i} = \langle i | m\rangle.$$

$$\therefore \langle n | m\rangle = \sum_{i} \langle n | i\rangle \langle j | m\rangle \langle i | j\rangle$$

$$= \sum_{i,j} \langle n | i\rangle \langle j | m\rangle \delta_{ij}$$

$$= \sum_{i} \langle n | i\rangle \langle i | m\rangle.$$

Problem 6. Calculate the sum over a complete orthonormal set $|i\rangle$, of the quantities $|\langle n | A | i \rangle|^2$. What value is obtained if A is unitary?

Sol.
$$\Sigma \mid \langle n \mid A \mid i \rangle \mid^2 = \Sigma \langle n \mid A \mid i \rangle \langle n \mid A \mid i \rangle^*$$

= $\Sigma \langle n \mid A \mid i \rangle \langle i \mid A \mid n \rangle$

$$= \langle n \mid AA\dagger \mid n \rangle$$

$$\{ : \mid i \} \text{ forms a complete set} \}$$

If A is unitary, then $AA\dagger = 1$ and hence we have

$$\sum_{i} |\langle n \mid A \mid i \rangle|^{2} = \langle n \mid n \rangle = 1.$$

Problem 7. Show that the projection operator Pi is Hermitian and positive definite.

Sol. For two arbitrary kets $|m\rangle$ and $|n\rangle$, we have $\langle n \mid P_i \mid m \rangle = \langle n \mid i \rangle \langle i \mid m \rangle$

 $= \langle m \mid i \rangle^* \langle i \mid n \rangle^*$ $= \langle m \mid P_i \mid n \rangle^*,$

i e. P. is Hermitian.

also we have

$$\langle n \mid P_i \mid n \rangle = \langle n \mid i \rangle \langle i \mid n \rangle = |\langle n \mid i \rangle|^2 \geqslant 0,$$

i.e., P_i is positive definite.

Problem 8. A projection operator Pi is said to be greater than or equal to another projection operator P1; if the space, in which P1 is defined as contained in the space, in which we define P, Show that

- (a) The relation $P_t \geqslant P_J$ satisfies the axioms required of any relation of inequality.
 - $[P_i P_j] = 0.$
- (c) The relation $P_1 \geqslant P_2$ is equivalent to the statement $\langle \psi \mid P_i \mid \psi \rangle \geqslant \langle \psi \mid P_j \mid \psi \rangle$ for any vector $|\psi \rangle$ of the Hilbert space.
- Sol. (a) From the definition it follows that, if $P_i \ge P_i$ and $P_i = P_i$ $P_1 \geqslant P_i$, then and that, if $P_i \geqslant P_j$ and $P_j \geqslant P_k$, then $P_i \geqslant P_k$.
 - (b) From the inequality, $P_i \geqslant P_j$, we have

$$P_i P_j \geqslant P_j^2 = P_j,$$
 ...(i)

$$P_j P_i \geqslant P_j^2 = P_j$$
, ...(ii)

$$P_i^2 = P_i \geqslant P_i P_j$$
, ...(iii)

and

$$P_i^2 = P_i \geqslant P_j P_i$$
 ...(iv)

From (i), on multiplying from left by P_i we get

$$P_i^2 P_j \geqslant P_i P_j$$

 $P_i P_i > P_i P_i$

or

$$P_i P_j \geqslant P_i P_j$$
.

From it we see that in (i) inequality sign cannot hold because that will give $P_iP_j > P_iP_j$ which is not possible. Hence the equality sign only is possible. Thus

Similarly, from (ii), (iii) and (iv), we have

$$P_j P_i = P_j$$
, ...(vi)

$$P_i = P_i P_j$$
 ...(vii)
 $P_i = P_j P_i$...(viii)

and

From (v) and (vi) or (vii), we have

 $P_{i}P_{j}=P_{j}P_{i},$

and hence

 $[P_i, P_j] = 0.$

(c) In general, for the projection operator P_i , we have, $P_i \mid \psi \rangle = C_i \mid \psi_i \rangle$

the component of ψ along the operator P_i .

If $|\psi\rangle$ belongs to the complementary-space of P_i , then

 $P_i \mid \psi \rangle = 0,$

and, in accordance with the relation $\langle \psi \mid P_i \mid \psi \rangle \geqslant \langle \psi \mid P_j \mid \psi \rangle$, we have $P_j \mid \psi \rangle = 0$.

Then, if $|\psi\rangle$ belongs to the space of P_j , $(1-P_i)|\psi\rangle=0$ and $P_j(1-P_i)|\psi\rangle=0$. If $|\psi\rangle$ does not belong to the space of P_i , $(1-P_i)|\psi\rangle=|\psi\rangle$. But $P_j|\psi\rangle=0$, and therefore for any $|\psi\rangle$ we have $P_j(1-P_i)|\psi\rangle=0$, and hence $P_j=P_jP_i$, which is equivalent to the inequality $P_i\geqslant P_j$.

Problem 9. Consider a set of vectors $|x\rangle$, in which x is a continuous index which can take all values in the interval (x_1, x_2) . Show that if the vectors $|x\rangle$ are orthonormal in the sense that $\langle x' | x \rangle = \delta(x'-x)$, then the operator

$$P = \int_{x_1}^{x_2} |x\rangle dx \langle x|$$

is the projection operator of the subspace spanned by the set of vectors $|x\rangle$.

Sol. For any arbitrary vector $|\psi(x)\rangle$, we have that

$$P \mid \psi(x) \rangle = \int_{x_1}^{x_2} \mid x' \rangle dx' \langle x' \mid \psi(x) \rangle$$

and hence

$$\langle x'' \mid P \mid \psi (x) \rangle = \int_{x_1}^{x_2} \langle x'' \mid x' \rangle dx' \langle x' \mid \psi (x) \rangle$$

$$= \int_{x_1}^{x_2} \delta(x'' - x') dx' \langle x' \mid \psi (x) \rangle$$

$$= \langle x'' \mid \psi (x) \rangle.$$

 $\langle x'' \mid (1-P) \mid \psi(x) \rangle = \langle x'' \mid \psi(x) \rangle - (x'' \mid P \psi(x) \rangle = 0.$...(i) Since $P \mid \psi(x) \rangle$ can be written as a linear combination of the $\mid x \rangle$ vectors, and from (i) we see that $(1-F) \mid \psi(x) \rangle$ is orthogonal to all of these vectors, it follows that P is a projection operator onto the subspace spanned by the $\mid x \rangle$ vectors.

Problem 10. Show that the matrix representation of a Hermitian operator is Hermitian.

Sol. If A is a Hermitian operator, then for any two given states ψ_i and ψ_i , we have

$$(\psi_i, A\psi_j) = A\psi_i, \psi_j. \qquad \dots (i)$$

Now,
$$a_{ij} = (\psi_i \ A\psi_j)$$

$$\therefore A\dagger = [a_{ij}]\dagger = [a_{ji}^*] = [(\psi_i, A\psi_i)^*] = [(A\psi_i, \psi_j)]$$

$$= [(\psi_i, A\psi_j)] \quad \{\text{using (i)}\}$$

$$= [a_{ij}] = A$$

Thus the matrix represention of a Hermitian operator is Hermitian.

Problem 11. Express the expectation value of an operator A in terms of its matrix elements a_{ij} .

Sol. The expectation value of A is defined as

$$\langle A \rangle = \langle \psi \mid A \mid \psi \rangle$$
.

Writing $|\psi\rangle$ in terms of the complete set of eigenkets $|\psi_{l}\rangle$ we have

$$| \psi \rangle = \sum_{i} C_{i} | \psi_{i} \rangle$$

$$\langle A \rangle = \sum_{i,j} C_{i} C_{j} \langle \psi_{i} | A | \psi_{j} \rangle$$

$$= \sum_{i,j} C_{i} C_{j} a_{ij}$$

This is the required expression.

Problem 12. Show that the matrix of the product of two operators is the product of the separate matrices representing the operators.

Sol. Let A and B be two operators with matrix elements a_{ij} and b_{ij} then

$$a_{ij} = \langle \psi_i \mid A \mid \psi_i \rangle$$
 ...(i)

and

$$b_{ij} = \langle \psi_i \mid B \mid \psi_j \rangle$$
 ...(ii)

Now, if we define the product AB as a matrix C, then $C_{i,j} = \langle \psi_i \mid AB \mid \psi_j \rangle = \sum_{k} \langle \psi_i \mid \psi_k \rangle A \mid \langle \psi_k \mid B \mid \psi_j \rangle$

$$\{:: \sum_{k} |\psi_{k}\rangle\langle\psi_{k}|=1 \text{ for the projection operator } |\psi_{k}\rangle\langle\psi_{k}|\}$$

$$= \sum_{k} a_{ik} b_{kj}$$

and hence the result.

Problem 13. Show by use of the bra-ket notation that trace $A=\Sigma \langle i \mid A \mid i \rangle$,

is independent of the basis | i> and that, trace AB=trace BA

Sol. Let us take another basis $|j\rangle$. Then the trace in this basis is given by,

trace
$$A = \sum_{j} \langle j \mid A \mid j \rangle$$

Using the projection operator $|i\rangle\langle i|$, we can it as:

Using the projection projection
$$\Sigma$$
 $\langle j \mid A \mid j \rangle = \Sigma \langle j \mid i \rangle \langle i \mid A \mid i \rangle \langle i \mid j \rangle$

$$= \Sigma \langle i \mid A \mid i \rangle \langle j \mid i \rangle \langle i \mid j \rangle$$

$$= \Sigma \langle i \mid A \mid i \rangle \{ :: \Sigma \langle j \mid i \rangle \langle i \mid j \rangle = \Sigma \langle j \mid j \rangle = 1 \}$$

$$= \Sigma \langle i \mid A \mid i \rangle \{ :: \Sigma \langle j \mid i \rangle \langle i \mid j \rangle = \Sigma \langle j \mid j \rangle = 1 \}$$

Thus the trace A is independent of the basis.

Now,

trace
$$AB = \sum_{i} \langle i \mid AB \mid i \rangle$$

 $= \sum_{i} \langle i \mid A \mid i \rangle \langle i \mid B \mid i \rangle$
 $= \sum_{i} \langle i \mid B \mid i \rangle \langle i \mid A \mid i \rangle$
 $= \sum_{i} \langle i \mid BA \mid i \rangle$
 $= \text{trace } BA$.

Problem 14. Show that $\sum_{i,j} |\langle i, A | j \rangle|^2$ is independent of

the basis $|i\rangle$ and $|j\rangle$. (which need not be the same).

Sol.
$$\Sigma\Sigma \mid \langle i \mid A \mid j \rangle \mid^2 = \Sigma\Sigma \atop ij} \langle i \mid A \mid j \rangle \langle i \mid A \mid j \rangle^*$$

$$= \Sigma\Sigma \atop ij} \langle i \mid A \mid j \rangle \langle j \mid A \uparrow \mid i \rangle$$

$$= \Sigma \atop ij} \langle i \mid AA \uparrow \mid i \rangle$$

$$= \text{trace } AA \uparrow,$$

which is independent of the basis $|i\rangle$ and $|j\rangle$.

Problem 15. Starting from the eigenvalue equation, $A \mid \psi_i \rangle = \lambda_i \mid \psi_i \rangle$, A is unitary;

show that $\lambda_i = e^{ic}$, where C is a real constant, and hence prove the orthogonality of the eigenvectors of a unitary operator.

Sol. we have

$$A \mid \psi_i \rangle = \lambda_i \mid \psi_i \rangle$$

$$\langle \psi_i \mid A \uparrow = \lambda_i^* \langle \psi_i \mid$$

Hence,

$$\langle \psi_i \mid A \dagger A \mid \psi_i \rangle = \lambda_i * \lambda_i \langle \psi_i \mid \psi_i \rangle$$

or $\langle \psi_i | \psi_i \rangle = |\lambda_i|^2 \langle \psi_i | \psi_i \rangle \{ :: A \text{ is unitary, therefore, } A \dagger A = 1;$

Now the norm $\langle \psi_i | \psi_i \rangle \neq 0$ unless $| \psi_i \rangle$ is zero, therefore, $1 - |\lambda_i|^2 = 0$ or $|\lambda_i|^2 = 1 \Rightarrow \lambda_i = e^{ic}$; C is real.

To prove the orthogonality, let us consider another eigenvector $|\psi_i\rangle$ of A with eigenvalue

 $\lambda_i = e^{iC'}$; is real constant, not equal to C.

Now we have,

$$\langle \psi_i \mid \psi_j \rangle = \langle \psi_i \mid A \dagger A \mid \psi_j \rangle = \lambda_i * \lambda_j \langle \psi_i \mid \psi_j \rangle$$

$$= e^{i (C' - C)} \langle \psi_i \mid \psi_j \rangle$$

or

 $[1-e^{i(C'-C)}] \langle \psi_i | \psi_j \rangle = 0.$

The term inside the square bracket in the above cannot be zero unless C'=C, thus

$$\langle \psi_i \mid \psi_j \rangle = 0$$
;

i.e., eigenvectors of a unitary operator belonging to different eigenvalues are orthogonal to each other.

Problem 16. Let $|\psi\rangle$ and $|\phi\rangle$ be two vectors of finite norm.

Show that, $Tr(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$.

Sol. Let us represent $|\psi\rangle\langle\phi|$ by the operator A. Then

Trace
$$A = \sum_{i} \langle i \mid A \mid i \rangle$$

$$= \sum_{i} \langle i \mid \psi \rangle \langle \phi \mid i \rangle$$

$$= \sum_{i} \langle \phi \mid i \rangle \langle i \mid \psi \rangle$$

$$= \langle \phi \mid \psi \rangle.$$

Problem 17. If A is any linear operator, show that $A \dagger A$ is a positive-definite Hermitian operator whose trace is equal to the sum of the square moduli of the matrix elements of A in any arbitrary representation. Deduce that Trace $(A \dagger A) = 0$ if and only if A = 0.

Sol. For arbitrary kets $| \psi \rangle$ and $| \phi \rangle$, we have

$$\langle \psi \mid A \dagger A \mid \phi \rangle = \langle \phi \mid A \dagger A \mid \psi \rangle^* \qquad \{ : (A \dagger A) \dagger = A \dagger (A \dagger) \dagger = A \dagger A \}$$

This shows that $A \dagger A$ is Hermitian.

Now, taking $| \phi \rangle = | \psi \rangle$, and writing $| u \rangle = A | \psi \rangle$, we have that $\langle \psi | A \dagger A | \psi \rangle = \langle u | u \rangle \geqslant 0$;

and hence A†A is positive definite.

Now,
$$T_{\tau}(A \dagger A) = \sum_{i} \langle i \mid A \dagger A \mid i \rangle$$

$$= \sum_{i, j} \langle i \mid A \dagger \mid j \rangle \langle j \mid A \mid i \rangle$$

$$= \sum_{i, j} |\langle i \mid A \mid j \rangle|^{2} \geqslant 0$$

$$= \sum_{i, j} |\langle i \mid A \mid j \rangle|^{2} \geqslant 0$$

The equality is true only if all the elements $\langle i \mid A \mid j \rangle = 0$, which is equivalent to the operator relation A=0.

Problem 18. Show that a necessary and sufficient condition for two linear operators A and B to be equal (within a phase factor; i.e., $A=Be^{i\alpha}$) is that $|\langle \psi \mid A \mid \phi \rangle|=|\langle \psi \mid B \mid \phi \rangle$ for any pair of linearly independent kets $|\psi\rangle$ and $|\phi\rangle$.

Sol. To prove the necessity of the condition let us take, $A=Be^{i\alpha}$.

Then,
$$\langle \psi \mid A \mid \phi \rangle = e^{i\alpha} \langle \psi \mid B \mid \phi \rangle$$

or $|\langle \psi \mid A \mid \phi \rangle| = |e^{i\alpha} \langle \psi \mid B \mid \phi \rangle| = |\langle \psi \mid B \mid \phi \rangle|$...(i

To prove its sufficiency, let us consider a representation in which $a_{ij} = \langle i \mid A \mid j \rangle$ and $b_{ij} = \langle i \mid B \mid j \rangle$ are the matrix elements of the operators A and B. Taking $|\psi\rangle = |i\rangle$ and $|\phi\rangle = |j\rangle$ we have from (i) that,

$$|a_{ij}| = |b_{ij}|$$
 ...(ii)

for any $|i\rangle$ and $|j\rangle$. On the other hand, with $|\psi\rangle = |i\rangle$ and $|\phi\rangle = C_j |j\rangle + C_l |l\rangle$, where C_i and C_i are arbitrary complex numbers, we find from (i) that $|C_ja_{il}+C_la_{il}|=|C_jb_{ij}+C_lb_{il}|$...(iii)

Using (ii), we can write (iii) as

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$$Re \left[C_{j}C_{l}^{*}\left(a_{ij}a_{il}^{*}-b_{ij}b_{il}^{*}\right)\right]=0$$
 ...(iv)

Since the complex number $C_jC_i^*$ is arbitrary, it follows from (iv) that

$$a_{ij}a_{il}*-b_{ij}b_{il}*=0 \qquad ...(v)$$

From (ii) and (v) we now have,

$$\frac{a_{ij}}{b_{ij}} = \frac{a_{il}}{b_{il}}, \qquad \dots \text{(vi)}$$

which means that the ratio $\frac{a_{ij}}{b_{ij}}$ is independent of j.

On repeating the above arguments after interchanging rows and columns, we find that the ratio $\frac{a_{ij}}{b_{ij}}$ does not depend on i also. Hence from (ii) we can write that

$$\frac{a_{ij}}{b_{ij}} = e^{i\alpha}, \qquad \dots \text{(vii)}$$

where α is a real number independent of i and j; i.e., the two operators are equal to each other within a constant phase factor.

Problem 19. Given the matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -1 \\ i & 0 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Show that

- (a) These are Hermitian.
- Satisfy the relations $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I; \quad \sigma_x \sigma_y = i\sigma_z; \quad \sigma_y \sigma_z = i\sigma_x;$ $\sigma_z \sigma_x = i \sigma_y$; $\sigma_x \sigma_y - \sigma_y \sigma_x = 2i \sigma_z$; $\sigma_x \sigma_y + \sigma_y \sigma_x = 0$.
- Find the eigenvalues and normalized eigenvectors of these matrices.
- (d) Show that any arbitrary 2×2 matrix can be written as a linear combination of σ_x , σ_y , σ_z and I, the 2×2 unit matrix.
- Sol. (a) If the Hermitian conjugate of a matrix is equal to itself, it is called a Hermitian matrix. Now,

$$\sigma_{y}^{*} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}.$$

$$\therefore \quad \sigma_{y}^{*} + \tilde{\sigma_{y}^{*}} = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} = \sigma_{y}.$$

σy is Hermitian.

Similarly, we can show that σ_x and σ_z are also Hermitian.

Similarly, we can show that
$$\sigma_x$$
 and σ_z and σ_z are (b) $\sigma_x^2 = \sigma_x \cdot \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0.0 + 1.1 & 0.1 + 1.0 \\ 1.0 + 0.1 & 1.1 + 0.0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I.$

Similarly, $\sigma_y^2 = \sigma_z^2 = I$.

$$\sigma_{x}\sigma_{y} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0.0 + 1.i & 0. -i + 1.0 \\ 1.0 + 0.i & 1. -i + 0.0 \end{pmatrix} \\
= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i\sigma_{z}.$$

Similarly,
$$\sigma_y \sigma_z = i\sigma_x$$
 and $\sigma_z \sigma_x = i\sigma_y$,

$$\sigma_y \sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0.0 + (-i).1 & 0.1 + (-i).0 \\ i.0 + 0.1 & i.1 + 0.0 \end{pmatrix}$$

$$= \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} = -i\sigma_z.$$

 $\sigma_x \sigma_y - \sigma_y \sigma_x = i \sigma_z - (-i \sigma_z) = 2i\sigma_z$ $\sigma_x \sigma_y + \sigma_y \sigma_x = i \sigma_z + (-i \sigma_z) = 0.$

(c) We have found out the eigenvalues of the matrix σ_z (see section 36).

Similarly, one can find out the eigenvalues and the normalized eigenvectors for σ_x and σ_y .

For σ_x , we get

也也必要不是多少少。

$$\frac{1}{\sqrt{(2)}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
 for $\lambda = 1$ and $\frac{1}{\sqrt{(2)}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ for $\lambda = -1$.

For
$$\sigma_{\nu}$$
, we get

$$\frac{1}{\sqrt{(2)}} {1 \choose i}$$
 for $\lambda = 1$ and $\frac{1}{\sqrt{(2)}} {1 \choose -i}$ for $\lambda = -1$.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = C_1 \sigma_x + C_2 \sigma_y + C_3 \sigma_3 + C_4 I_3$$

 $\binom{a}{c} \binom{b}{d} = C_1 \sigma_x + C_2 \sigma_y + C_3 \sigma_3 + C_4 I,$ where $\binom{a}{c} \binom{b}{d}$ is an arbitrary given matrix and C_1 , C_2 , C_3 , C_4 are

unknown constants,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = C_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + C_2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + C_2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + C_4 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} C_3 + C_4 & C_1 - iC_2 \\ C_1 + iC_2 & -C_3 + C_4 \end{pmatrix} .$$

Therefore,
$$C_3 + C_4 = a$$

$$C_1 - iC_2 = b$$

$$C_1 + iC_2 = c$$

$$C_1 + iC_2 = c$$

$$-C_3 + C_4 = d$$

$$C_1 = \frac{1}{2} (b + c),$$

$$C_2 = \frac{1}{2} (a - b),$$

$$C_3 = \frac{1}{2} (a - d),$$

$$C_4 = \frac{1}{2} (a + d).$$

Hence we can write for an arbitrary 2×2 matrix as

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{2} (b+c) \sigma_x + \frac{1}{2i} (c-b) \sigma_y + \frac{1}{2} (a-d) \sigma_z + \frac{1}{2} (a+d) I.$$

Problem 20. Prove that a necessary and sufficient condition for A to be unitary is that for every vector $|i\rangle$, $\langle i | A \dagger A | i\rangle = \langle i | i\rangle$. Hence show that every eigenvalue of a unitary matrix has absolute magnitude unity.

Sol. To prove the necessity, let us suppose that A is unitary. Then $A\dagger A = I$ and hence we have,

$$\langle i \mid A \dagger A \mid i \rangle = \langle i \mid I \mid i \rangle = \langle i \mid i \rangle.$$

On the other hand, for sufficiency, we have

$$\langle i \mid A \dagger A \mid i \rangle = \langle i \mid i \rangle$$

 $\Rightarrow A \dagger A = I \text{ in the representation } | i \rangle.$

If we show that $A\dagger A=I$ in any representation, then we can say that A is unitary. Now the transformation from one representation to another is made by a unitary matrix U in the following way,

$$A^{(1)} = U \dagger AU, \ A^{(1)} \dagger = U \dagger A \dagger U.$$

Hence it follows that

$$A^{(1)}\dagger A^{(1)} = U\dagger A\dagger UU\dagger AU = I$$

 $\Rightarrow A \dagger A = I$ in any representation.

The fact that every eigenvalue of a unitary matrix has absolute magnitude unity had already been proved in problem 15.

Problem 21. Prove that the matrices

$$A = \begin{cases} -\frac{1}{3} & \sqrt{\left(\frac{2}{3}\right)} & \frac{\sqrt{(2)}}{3} \\ \sqrt{\left(\frac{2}{3}\right)} & 0 & \frac{1}{\sqrt{(3)}} \\ \frac{\sqrt{(2)}}{3} & \frac{1}{\sqrt{(3)}} & -\frac{2}{3} \end{cases}; B = \begin{cases} \frac{5}{3} & \frac{1}{\sqrt{(6)}} - \frac{1}{3\sqrt{(2)}} \\ \frac{1}{\sqrt{(6)}} & \frac{3}{2} & \frac{1}{2\sqrt{(3)}} \\ -\frac{1}{3\sqrt{(2)}} & \frac{1}{2\sqrt{(3)}} & \frac{11}{6} \end{cases}$$

satisfy the equation

$$(I+A)(2I-B)=0.$$

What is the significance of this equation relative to the simultaneous eigen vectors of A and B?

Sol. It can very easily be seen by using matrix addition and multiplication that

Now
$$(I+A) (2I-B)=0.$$

 $(I+A) (2I-B)=2I-B+2A-AB$
and $(2I-B)(I+A)=2I-B+2A-BA.$

From these equations we see that if A and B have simultaneous eigenvectors, then

$$(I+A)(2I-B) = (2I-B)(I+A) = 0$$
 {: $AB=BA$ }

i.e., (I+A) and (2I-B) also have simultaneous eigenvectors, if A and B have simultaneous eigenvectors.

Problem 22. Let $\psi(x)$ be a column vector whose components are analytic functions of a parameter x:

$$\psi(x) = \begin{bmatrix} C_1(x) \\ C_2(x) \\ \vdots \\ C_n(x) \end{bmatrix}$$

and let $\frac{d\psi(x)}{dx} = \lim_{h \to 0} \frac{\psi(x+h) - \psi(x)}{h}$ be the derivative of $\psi(x)$.

Then prove that if

$$\frac{d\psi(x)}{dx} = A\psi(x),$$

where A is a matrix independent of x, then

$$\psi(x) = e^{(x-x_0)} A_{\psi(x_0)},$$

where x_0 is some fixed value of x.

Sol. We have

$$\frac{d\psi(x)}{dx} = A\psi(x). \qquad \therefore \quad \frac{d\psi(x)}{\psi(x)} = A \ dx.$$

Integrating both sides w.r.t. x, we get

 $\log \psi(x) = Ax + C$, where C is the constant of integration.

For $x=x_0$, we have

$$\log \psi(x_0) = Ax_0 + C.$$

$$C = \log \psi(x_0) - Ax_0.$$

Using this value of C, we obtain

$$\log \psi(x) = Ax + \log \psi(x_0) - Ax_0$$

or
$$\log \psi(x) - \log \psi(x_0) = (x - x_0) A$$

or
$$\log \frac{\psi(x)}{\psi(x_0)} = (x - x_0) A$$
$$\Rightarrow \frac{\psi(x)}{\psi(x_0)} = e^{(x - x_0) A}$$

$$\psi(x_0) = e^{(x-x_0)A} \psi(x_0).$$

Problem 23. Construct the products AB and BA of the infinite matrices

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ & & \text{etc.} \end{bmatrix} = [\delta_i, j-1]; B = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ & & & \text{etc.} \end{bmatrix} = [\delta_i, j+1].$$

Does either A or B have an inverse?

Sol. Let us call AB=C and BA=D, then the *ij*-th element C_{ij} of AB is given by:

$$C_{i,} = \sum_{k=1}^{\infty} a_{ik} b_{kj} = \sum_{k=1}^{\infty} \delta_{i}, k_{-1} \delta_{k}, j+1$$

= $\delta_{i}, (j+1)-1 = \delta_{ij}$

and

$$d_{ij} = \sum_{k=1}^{\infty} b_{ik} \ a_{kj} = \sum_{k=1}^{\infty} \delta_{i}, \ k+1 \ \delta_{k}, \ j-1$$
$$= \delta_{i}, \ (j-1)+1 = \delta_{ij}$$

:. $AB = BA = [\delta_{ij}]$, the unit matrix of infinite order.

Thus A and B are inverse of each other.

Problem 24. If $B=e^A$, then show that

$$det. B = e^{trace A},$$

where A is a diagonalizable matrix.

Sol. Because A is diagonalizable, by a similarity transformation of A we can get a matrix Λ which is a diagonal matrix; i.e.,

$$U^{-1} A U = \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 & \dots \\ 0 & \lambda_2 & 0 & \dots \\ 0 & 0 & \lambda_3 & \dots \\ & & \text{etc.} \end{bmatrix}$$

We can write,

$$A = U\Lambda U^{-1}$$

$$\therefore \text{ exp. } A = I + A + \frac{A^{2}}{2!} + \dots$$

$$= UU^{-1} + U\Lambda U^{-1} + \frac{1}{2!} U\Lambda U^{-1} U\Lambda U^{-1} + \dots$$

$$= U \left[I + \Lambda + \frac{\Lambda^{2}}{2!} + \dots \right] U^{-1}$$

$$= U \text{ (exp. } \Lambda) U^{-1}$$

Hence,

det. (exp.
$$A$$
)=(det U) det (exp. Λ) (det U^{-1})=det (exp. Λ)
=(exp λ_1) (exp. λ_2) (exp λ_3)...
=exp ($\lambda_1+\lambda_2+...+\lambda_n$)
=exp (trace Λ)=exp (trace A).

trace of a matrix does not change under similarity transformation}

 \therefore det $B=e^{\operatorname{trace} A}$.

Problem 25. Show that the eigenvalues of a Hermitian matrix are real.

Suppose A is a Hermitian matrix and λ is an eigenvalue of it with non-zero eigenvector $|\psi\rangle$,

$$A \mid \psi \rangle = \lambda \mid \psi \rangle$$
 ...(i)
 $\langle \psi \mid A \uparrow = \lambda^* \langle \psi \mid$ {:: A is Hermitian} ...'ii)

From (i) and (ii) we have

$$\langle \psi \mid A \mid \psi \rangle = \lambda \langle \psi \mid \psi \rangle$$

and
$$\langle \psi \mid A \mid \psi \rangle = \lambda^* \langle \psi \mid \psi \rangle$$
; respectively.

Comparing these we have, $\lambda^* = \lambda$, i.e., λ is real.

Problem 26. Show that eigenvectors of a Hermitian matrix belonging different eigenvalues are orthogonal.

Sol. Let A be a Hermitian matrix with eigenvector $|\psi_i\rangle$ and $|\psi_{i}\rangle$ such that,

$$A \mid \psi_i \rangle = \lambda_i \mid \psi_i \rangle$$
; $A \mid \psi_j \rangle = \lambda_j \mid \psi_j \rangle$ and $\lambda_i \neq \lambda_j$.

From these equations we have,

$$\langle \psi_i \mid A = \lambda_i \langle \psi_j \mid \text{and } \langle \psi_j \mid A = \lambda_j \langle \psi_j \mid A \rangle$$

 $\langle \psi_i \mid A \mid \psi_j \rangle = \lambda_i \langle \psi_i \mid \psi_j \rangle$

 $\langle \psi_i \mid A \mid \psi_j \rangle = \lambda_j \langle \psi_i \mid \psi_j \rangle$

Subtracting these, we have

$$0 = (\lambda_i - \lambda_j) \langle \psi_i | \psi_j \rangle$$

$$\Rightarrow \langle \psi_i | \psi_j \rangle = 0 \quad (:: \lambda_i \neq \lambda_j)$$

i.e., $|\psi_i\rangle$ and $|\psi_j\rangle$ are orthogonal.

Problem 27. Show that a Hermitian matrix remains Hermitian under a unitary transformation.

Sol. Suppose the Hermitian matrix $A^{(1)}$ is transformed into the matrix $A^{(2)}$ by the unitary transformation U; i.e.,

$$A^{(2)} = U^{-1} A^{(1)} U$$

Transposing, $\tilde{A}^{(2)} = \tilde{U} \tilde{A}^{(1)} \tilde{U}^{-1}$ As the matrix U is unitary and $A^{(1)}$ is Hermitian, therefore,

$$\tilde{A}^{(2)} = (U^{-1} A^{(1)} U)^* = A^{(2)*}$$

Hence, A(2) is also Hermitian.

Problem 28. Show that, if the operators A, B and C satisfy the commutation relation [A, B] = iC in the Schroedinger picture, this relation is valid in the other pictures also.

Sol. We have in the Heisenberg picture,

$$A_{H} = e^{iHt/\hbar} A e^{-iHt/\hbar}$$

$$B_{H} = e^{iHt/\hbar} B e^{-iHt/\hbar}$$

$$\vdots [A_{H}, B_{H}] = A_{H}B_{H} - B_{H}A_{H}$$

$$= e^{iHt/\hbar} A e^{-iHt/\hbar} e^{iHt/\hbar} B e^{-iHt/\hbar}$$

$$-e^{-iHt/\hbar} B e^{-iHt/\hbar} e^{iHt/\hbar} A e^{-iHt/\hbar},$$

$$= e^{iHt/\hbar} A B e^{-iHt/\hbar} - e^{iHt/\hbar} B A e^{-iHt/\hbar},$$

$$= e^{iHt/\hbar} (AB - BA) e^{-iHt/\hbar},$$

$$= e^{iHt/\hbar} iC e^{-iHt/\hbar},$$

$$= e^{iHt/\hbar} iC e^{-iHt/\hbar},$$

Similarly, $[A_I, B_I] = iC_I$.

Problem 29. Treating the coordinate x as an operator in the Schroedinger picture, determine the corresponding operator x_H in the Heisenberg picture:

- (i) for a free particle and
- (ii) for the harmonic oscillator.

Sol. (i) For a free-particle,

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}.$$

$$\dots(i)$$

Now, $x_H = e^{iHt/\hbar} x_e - iHt/\hbar$

$$=x+\frac{it}{\hbar}[H,x]+\frac{1}{2!}\left(\frac{it}{\hbar}\right)^{2}[H,[H,x]]+... ...(ii)$$

$$\left\{ : e^{kB} Ae^{-kB}=A+k[B,A]+\frac{k^{2}}{2};[B,[B,A]]+... \right\}$$

From (i) we have,

$$[H, x] \psi (x) = -\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} (x \psi (x)) - x \frac{\partial^2}{\partial x^2} \psi (x) \right] = -\frac{\hbar^2}{m} \frac{\partial \psi(x)}{\partial x}.$$

$$\therefore [H, x] = -\frac{\hbar^2}{m} \frac{\partial}{\partial x}.$$

$$[H, [H, x]] = 0,$$

$$[H, [H, [H, x]]] = 0,...$$

$$(iii)$$

Using these commutators we find from (ii) that

$$x_H = x - \frac{i\hbar}{m} t \frac{\partial}{\partial x} \qquad ...(iv)$$

(ii) For the harmonic oscillator,

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2}$$

$$\therefore [H, x] = -\frac{\hbar^2}{2m} \frac{\partial}{\partial x}$$

$$[H, [H, x]] = \hbar^2 \omega^2 x; [H, [H, [H, x]]] = -\frac{\hbar^4 \omega^2}{m} \frac{\partial}{\partial x}$$

$$[H, [H, [H, [H, x]]]] = \hbar^4 \omega^4 x \text{ and so on.}$$

$$(V)$$

Hence we have,

$$x_{H} = x + \frac{it}{\hbar} \cdot \frac{-\hbar^{2}}{m} \frac{\partial}{\partial x} + \frac{1}{2!} \left(\frac{it}{\hbar}\right)^{2} \cdot \hbar^{2} \omega^{2} x$$

$$+ \frac{1}{3!} \left(\frac{it}{\hbar}\right)^{3} \cdot \frac{-\hbar^{4} \omega^{2}}{m} \frac{\partial}{\partial x} + \frac{1}{4!} \left(\frac{it}{\hbar}\right)^{4} \cdot \hbar^{4} \omega^{4} x + \dots$$

$$= x \left[1 - \frac{(\omega t)^{2}}{2!} + \frac{(\omega t)^{6}}{4!} - \dots\right] - \frac{i\hbar}{m\omega} \frac{\partial}{\partial x} \left[\omega t - \frac{(\omega t)^{3}}{3!} + \dots\right]$$

$$= x \cos \omega t - \frac{i\hbar}{m\omega} \sin \omega t \cdot \frac{\partial}{\partial x} \qquad \dots \text{(vi)}$$

Using $p = -i\hbar \frac{\partial}{\partial x}$, we can write (iv) and (vi) as:

$$x_H = x + \frac{p}{m} t$$
 for a free particls

and $x_H = x \cos \omega t + \frac{p}{m\omega} \sin \omega t$ for harmonic oscillator.

Problem 30. Construct the matrix of transformation in two dimensional Cartesian coordinate space, which doubles the legath of every vector drawn from the origin and rotates it through a positive angle of 45° . Show that this matrix satisfies the equation $A^{\bullet} = -16I$.

Sol. Let us consider a vector, $\begin{bmatrix} x \\ y \end{bmatrix}$ in the given space, which is transformed into the vector $\begin{bmatrix} x' \\ y' \end{bmatrix}$. The required transformation can be performed in two steps. First, rotate the given vector through 45° and then double its length.

If $\begin{bmatrix} x \\ y \end{bmatrix}$ makes an angle θ with the x-axis and if it is transformed into $\begin{bmatrix} x'' \\ y'' \end{bmatrix}$ by a rotation through 45° without any change in its length 'l', then

$$x = l \cos \theta, \quad y = l \sin \theta$$

$$x'' = l \cos (\theta + 45^{\circ}) = \frac{1}{\sqrt{2}} (l \cos \theta - l \sin \theta) = \frac{1}{\sqrt{2}} (x - y)$$

$$y'' = l \sin (\theta + 45^{\circ}) = \frac{1}{\sqrt{2}} (l \sin \theta + l \cos \theta) = \frac{1}{\sqrt{2}} (x + y)$$

In matrix form it can be written as

$$\begin{bmatrix} x'' \\ y'' \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \qquad \dots (i)$$

Now, for doubling the length we should have $x'' \rightarrow 2x''$ and $y'' \rightarrow 2y''$. Thus the final transformed vector $\begin{bmatrix} x' \\ y' \end{bmatrix}$ is given by

$$x' = 2x''$$
 and $y' = 2y''$

In matrix form it can be written as

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = 2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x'' \\ y'' \end{bmatrix} \qquad \dots (ii)$$

Using (i) into (ii), we get

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \sqrt{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \sqrt{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \dots \text{(iii)}$$

Thus the transformation matrix A is given by

$$A = \sqrt{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$
 ...(iv)

It is now easy to show that, $A^4 = -16 I$.

Problem 31. If $H = \hbar \omega$ ($aa\dagger + \frac{1}{2}$), where a and $a\dagger$ satisfy the commutation relation $a\dagger a - aa\dagger = 1$ then show that, $H^n a = a (H + \hbar \omega)^n$.

[Hint: Prove it by mathematical induction]

Problem 32. If $a(t) = e^{iHt/\hbar} a(0) e^{-iHt/\hbar}$, then show that $a(t) = a(0) e^{i\omega t}$

Sol.
$$a(t) = \left(1 + \frac{iHt}{\hbar} + \frac{i^2H^2t^2}{2!\hbar^2} + \frac{i^3H^3t^8}{3!\hbar^2} + \dots\right)a(0) e^{-iHt/\hbar}$$

$$= a(0) \left(1 + \frac{i(H + \hbar \omega)t}{\hbar} + \frac{i^2(H + \hbar \omega)^2 t^2}{2! \hbar^2} + \dots \right) e^{-iHt/\hbar}$$

$$= a(0) e^{i(H + \hbar \omega)t/\hbar} e^{-iHt/\hbar}$$

$$= a(0) e^{i\omega t}$$

Problem 33. Show that for a simple harmonic oscillator:

(a)
$$(E_l - E_k) \langle k \mid x \mid l \rangle = \frac{i\hbar}{m} \langle k \mid p \mid l \rangle$$
, and

(b) $\langle l \mid xp+px \mid l \rangle = 0$.

Sol. (a) We have the Hamiltonion for the oscillator as:

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$$

$$\therefore xH - Hx = \frac{i\hbar}{m} p \qquad ...(i$$

Taking the matrix element of both sides of it between the k-th and l-th states of the oscillator, we have—

or
$$\langle k \mid x \mid H - Hx \mid l \rangle = \frac{i\hbar}{m} \langle k \mid p \mid l \rangle$$
or
$$\langle k \mid xH \mid l \rangle - \langle k \mid Hx \mid l \rangle = \frac{i\hbar}{m} \langle k \mid p \mid l \rangle$$
or
$$E_{l} \langle k \mid x \mid l \rangle - E_{k} \langle k \mid x \mid l \rangle = \frac{i\hbar}{m} \langle k \mid p \mid l \rangle$$
or
$$(E_{l} - E_{k}) \langle k \mid x \mid l \rangle = \frac{i\hbar}{m} \langle k \mid p \mid l \rangle.$$

(b) From eq. (i) we have.

$$p = \frac{m}{i\hbar} (xH - Hx)$$

$$\langle k \mid xp + px \mid l \rangle = \frac{m}{i\hbar} \langle k \mid x (xH - Hx) + (xH - Hx)x \mid l \rangle$$

$$= \frac{m}{i\hbar} \langle k \mid x^2 H - xHx + xHx - Hx^2 \mid l \rangle$$

$$= \frac{m}{i\hbar} \langle k \mid x^2H - Hx^2 \mid l \rangle$$

$$= \frac{m}{i\hbar} \langle k \mid x^2H - Hx^2 \mid l \rangle$$

$$= \frac{m}{i\hbar} \langle E_1 - E_k \rangle \langle k \mid x^2 \mid l \rangle$$

Taking k=1 in the above eq. we get,

in the above eq. we get:
$$\langle l \mid xp + px \mid l \rangle = \frac{m}{i\hbar} (E_i - E_l) \langle l \mid x^2 \mid l \rangle = 0.$$

Problem 34. Show that for an oscillator transition from an initial state $|l\rangle$ with energy E_l to a final state $|k\rangle$ energy E_k we have,

$$\Sigma (E_{k}-E_{l}) | \langle k | x | l \rangle |^{2} = \frac{\hbar^{2}}{2m}$$
Sol.
$$\Sigma (E_{k}-E_{l}) | \langle k | x | l \rangle |^{2} = \Sigma (E_{k}-E_{l}) \langle l | x | k \rangle \langle k | x | l \rangle$$

$$= \Sigma [\langle l | xH | k \rangle - \langle l | Hx | k \rangle] \langle k | x | l \rangle$$

$$= \sum_{k} \langle l | xH-Hx | k \rangle \langle k | x | l \rangle$$

$$= \frac{i\hbar}{m} \sum_{k} \langle l | p | k \rangle \langle k | x | l \rangle$$

$$= \frac{i\hbar}{m} \langle l | px | l \rangle \qquad \dots (i)$$

Now,

$$\langle l \mid px \mid l \rangle = \frac{1}{2} \langle l \mid px - xp + xp + px \mid l \rangle$$

$$= \frac{1}{2} \langle l \mid px - xp \mid l \rangle + \frac{1}{2} \langle l \mid xp + px \mid l \rangle$$

$$= \frac{-i\hbar}{2} \langle l \mid l \rangle + 0 = \frac{-i\hbar}{2}. \qquad ...(ii)$$

$$\therefore \sum_{k} (E_{k} - E_{l}) |\langle k | x | l \rangle|^{2} = \frac{i\hbar}{lm} \cdot \frac{-i\hbar}{2} = \frac{\hbar^{2}}{2m} \cdot \dots \text{(iii)}$$

$$\therefore \sum_{k} (E_{k} - E_{l}) |\langle k | x | l \rangle|^{2} = \frac{i\hbar}{lm} \cdot \frac{-i\hbar}{2} = \frac{\hbar^{2}}{2m} \cdot \dots \text{(iii)}$$

$$\therefore \sum_{k} (E_{k} - E_{l}) |\langle k | x | l \rangle|^{2} = \frac{i\hbar}{lm} \cdot \frac{-i\hbar}{2} = \frac{\hbar^{2}}{2m} \cdot \dots \text{(iii)}$$

This relation is known as Thomas-Reiche-Kuhn sum rule. It can be used for atomic excitations if we recognize 'x' by the x-component of the total dipole moment operator.

We have seen that the physical state of a particle at time 't' is described as fully as possible by the normalized wavefunction $\psi(\mathbf{r}, t).P(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$ gives the probability density for finding the particle at position r. The average (or expectation) values of position and momentum can be calculated from the wavefunction $\psi(\mathbf{r}, t)$ by the formulae,

$$\langle \mathbf{r} \rangle = \int \psi^* (\mathbf{r}, t) \, \mathbf{r} \psi(\mathbf{r}, t) \, d^3 r, \qquad \dots (1-a)$$

$$\langle \mathbf{p} \rangle = \int \psi^* (\mathbf{r}, t) \, \mathbf{p} \, \psi(\mathbf{r}, t) \, d^3 r$$

$$= \int \psi^* (\mathbf{r}, t) \, (-i\hbar) \, \nabla \psi(\mathbf{r}, t) \, d^3 r. \qquad \dots (1-b)$$

The development of $\psi(\mathbf{r}, t)$ with time is governed by the Schroedinger's equation of motion

$$\left(-\frac{\tilde{y}^2}{2m}\nabla^2 + V\right)\psi = i\hbar \frac{\partial \psi}{\partial t}. \qquad ...(2)$$

Now we assert that a significant progress in the understanding of Quantum Mechanics can be made by making a Fourier transform of the wavefunction $\psi(\mathbf{r}, t)$. Before exploring such significance, we first recall the elements of the Fourier analysis.

4.1. ELEMENTS OF FOURIER ANALYSIS:

The Fourier transform of any algebraic function $\psi(x)$ is given by

$$\psi(x) = \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} a(k) e^{ikx} dk, \qquad \dots (3-a)$$

where the coefficients a(k) are known as the Fourier components of $\psi(x)$ and these are given by

$$a(k) = \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} \psi(x) \ e^{-ikx} \ dx. \qquad ...(3-b)$$

Putting the value of a(k) from (3-b) in (3-a), we get

ing the value of
$$u(x)$$
 from $\psi(x) = \frac{1}{\{\sqrt{(2\pi)}\}^2} \int_{-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} \psi(x') e^{-ikx'} dx' \right) e^{ikx} dk$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi(x') e^{ik(x-x')} dx' dk. \qquad ...(4)$$

Equation (4) is called the Fourier Integral Theorem. It is conventional to define the Dirac delta function $\delta(x)$ by

conventional to define the Dirac define
$$\delta(0) = \infty$$
, $\delta(x) = 0$ if $x \neq 0$:
$$\int_{-\infty}^{+\infty} \delta(x) dx = 1, \qquad \dots (5)$$

$$\delta(0) = \infty, \delta(x) = 0 \text{ if } x \neq 0 : \int_{-\infty}^{+\infty} \delta(x) dx = 1, \qquad \dots (5)$$

where the region of integration includes the point x=0. An equivalent definition is that, for an arbitrary function $\psi(x)$, the equation

$$\int_{-\infty}^{+\infty} \psi(x') \, \delta(x - x') \, dx' = \psi(x) \qquad \dots (6)$$

is valid, where the range of integration includes the point x.

Comparing (4) with (6), we can write
$$\delta(x-x') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(x-x')} dk. \qquad ...(7)$$

Now we use this definition of delta function to evaluate the important integral,

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx,$$

in terms of the Fourier components of $\psi(x)$.

We write,
$$\int_{-\infty}^{+\infty} |\psi(x)|^{2} dx = \int_{-\infty}^{+\infty} \left[\left\{ \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} a^{*}(k) e^{-ikx} dk \right\} \right] \times \left\{ \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} a(k') e^{ik' x} dk' \right\} dx$$

$$= \int_{-\infty}^{+\infty} dk \, a^{*}(k) \int_{-\infty}^{+\infty} dk' \, a(k') \cdot \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i(k'-k) x} dx$$

$$= \int_{-\infty}^{+\infty} dk \, a^{*}(k) \int_{-\infty}^{+\infty} dk' \, a(k') \, \delta(k'-k)$$

$$= \int_{-\infty}^{+\infty} |a(k)|^{2} dk. \qquad ...(8)$$

Equation (8) is written by carrying out the integral over k' by using the definition (6) of the delta function. It is known as the Parseval's formula.

Generalizing equations (3), we may write for the Fourier transforms of the wavefunction $\psi(\mathbf{r}, t)$ as

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi(\mathbf{p}, t) e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} d^3p \qquad \dots (9-a)$$

and

$$\phi(\mathbf{p}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\mathbf{r}, t) e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} d^3r \qquad \dots (9-b)$$

We have written these equations in terms of the momentum p rather than the propagation vector k. The relation between the two is

p=ħk

For it, the Parseval's formula is generalized to the form:

$$\int |\psi(\mathbf{r}, t)|^2 d^3r = \int |\phi(\mathbf{p}, t)|^2 d^3p \qquad ...(10)$$

The delta function can also be defined for the three dimensional case as:

se as:

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3} \int e^{i\mathbf{k}.\mathbf{r}} d^3k = \frac{1}{(2\pi\hbar)^3} \int e^{i\mathbf{p}.\mathbf{r}/\hbar} d^3p \qquad ...(11)$$

4.2. MOMENTUM EIGENFUNCTIONS:

Let us consider the Schroedinger equation for a free particle,

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi. \qquad \dots (12)$$

It can be separated into three one dimensional equations by assuming a solution of the form,

$$\psi = X(x) \cdot Y(y) \cdot Z(z) \qquad \dots (13)$$

Taking $k^2 = k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2}$, we get the solutions of the form,

$$X(x) = Ae^{ik_x x} + Be^{-ik_x x}$$

$$Y(y) = Ce^{ik_y y} + De^{-ik_y y}$$

$$Z(z) = Fe^{ik_z z} + Ge^{-ik_z z}$$

$$(14)$$

Considering only the first terms (the second terms are obtained by simply changing the sign of (k_x, k_y, k_z) , eqns. (14) can be written as:

$$\psi = Ne^{i(k_x x + k_y y + k_z z)}$$

$$= Ne^{ik.r}. \qquad ...(15)$$

N is the normalization constant and k is the propagation vector. Solution (15) is known as the momentum eigenfunction because it is an eigenfunction of the operator for the linear momentum, $\mathbf{p} = -i\hbar \nabla$, having the eigenvalue $\hbar \mathbf{k}$,

$$\mathbf{p}\psi = -i\hbar \nabla e^{i\mathbf{k}\cdot\mathbf{r}} = -i\hbar \left(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right) e^{i\left(k_x x + k_y y + k_z z\right)}$$

$$= \hbar \mathbf{k} \psi.$$

Solution (15) can be written in terms of momentum vector p
as:

 $\psi = Ne^{i\mathbf{p} \cdot \mathbf{r}/\hbar} \qquad \dots (17)$

4.3. SIGNIFICANCE OF THE FOURIER TRANSFORMS $\phi(p, t)$:

In order to find out the significance of the Fourier Transforms $\phi(\mathbf{p}, t)$, we start with the evaluation of the average values of the position and the momentum operators as:

$$\langle \mathbf{p} \rangle = \int \psi^{*}(\mathbf{r}, t) \, \mathbf{p} \, \psi(\mathbf{r}, t) \, d^{3}r$$

$$= \int d^{3}r \, \frac{1}{(2\pi \hbar)^{3/2}} \int d^{3}p \phi^{*}(\mathbf{p}, t)$$

$$\times e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \mathbf{p} \, \frac{1}{(2\pi \hbar)^{3/2}} \int d^{3}p' \phi(\mathbf{p}', t) \, e^{i\mathbf{p}' \cdot \mathbf{r}/\hbar}$$

$$= \int d^{3}p \phi^{*}(\mathbf{p}, t) \, \mathbf{p} \, \int d^{3}p' \phi(\mathbf{p}', t) \, \frac{1}{(2\pi \hbar)^{3}} \int e^{i \, (\mathbf{p}' - \mathbf{p}) \cdot \mathbf{r}/\hbar} \, d^{3}r$$

$$= \int d^{3}p \phi^{*}(\mathbf{p}, t) \, \mathbf{p} \, \int d^{3}p' \phi(\mathbf{p}', t) \, \delta(\mathbf{p}' - \mathbf{p}).$$

$$= \int d^{3}p \phi^{*}(\mathbf{p}, t) \, \mathbf{p} \, \phi(\mathbf{p}, t) \quad ...(18)$$
and
$$\langle \mathbf{r} \rangle = \int d^{3}r \, \left[\frac{1}{(2\pi \hbar)^{3/2}} \int d^{3}p \phi^{*}(\mathbf{p}, t) \right]$$

$$\times e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \, \frac{1}{(2\pi \hbar)^{3/2}} \int d^{3}p' \phi(\mathbf{p}', t) \, \mathbf{r} \, e^{i\mathbf{p}' \cdot \mathbf{r}/\hbar} \, d^{3}p$$

$$= \int d^{3}r \, \left[\frac{1}{(2\pi \hbar)^{3/2}} \int \phi^{*}(\mathbf{p}, t) \, e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \, d^{3}p \right]$$

$$= \int d^{3}r \, \left[\frac{1}{(2\pi \hbar)^{3/2}} \int \phi^{*}(\mathbf{p}, t) \, e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \, d^{3}p \right]$$

$$= \int d^{3}r \, \left[\frac{1}{(2\pi \hbar)^{3/2}} \int \phi^{*}(\mathbf{p}, t) \, e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \, d^{3}p \right]$$

Here, $\nabla_{p'} = \hat{i} \frac{\partial}{\partial p_x} + \hat{j} \frac{\partial}{\partial p_y} + \hat{k} \frac{\partial}{\partial p_z}$, is the del operator in the momentum space.

or
$$\langle \mathbf{r} \rangle = \int d^3p \phi^* (\mathbf{p}, t) \int d^3p' (i\hbar \nabla_{p'}) \phi(\mathbf{p'}, t)$$

$$\times \frac{1}{(2\pi\hbar)^3} \int e^{i (\mathbf{p'} - \mathbf{p}) \cdot \mathbf{r}/\hbar} d^3r$$

$$= \int d^3p \phi^* (\mathbf{p}, t) \int d^3p' (i\hbar \nabla_{p'}) \phi(\mathbf{p'}, t) \delta(\mathbf{p'} - \mathbf{p})$$

$$= \int d^3p \, \phi^* \left(\mathbf{p}, \, t \right) \, i \, \mathbf{h} \, \nabla_{\mathbf{p}} \, \phi(\mathbf{p}, \, t). \qquad \dots (19)$$

Since $e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$ represents an eigenfunction of the momentum operator $(-i\hbar \nabla)$ with the momentum eigenvalue p; i.e., it represents a state of definite momentum p, therefore, according to eqn. (9-a), $\phi(\mathbf{p},t)$ is the amplitude with which the momentum \mathbf{p} appears in the state $\psi(\mathbf{r}, t)$. If $\phi(\mathbf{p}, t)$ is strongly peaked near a particular value of p, the state $\psi(\mathbf{r}, t)$ tends to be one of definite momentum. Combining this fact with eqn. (18) we conclude that $|\phi(\mathbf{p},t)|^2 = \phi^*(\mathbf{p},t) \phi(\mathbf{p},t)$ is the probability density for finding the momentum of the particle in the neighbourhood of p. There is great similarity between (1-a), (18) and (1-b), (19). Thus the wavefunction $\psi(\mathbf{r}, t)$ in position coordinate space and $\phi(\mathbf{p}, t)$ in momentum space, are both equally valid descriptions of the state of a system. Given either of them, the other can be evaluated from eqns. (9). From (10) we can also see that, if $\psi(\mathbf{r}, t)$ is normalized for some 't' in the coordinate space, $\phi(p, t)$ is automatically normalized in the momentum space.

When we work with $\psi(\mathbf{r}, t)$, we have what is called a position representation, and when we work with $\phi(p, t)$ it is called a momentum representation. Which of these representations is used is simply a matter of our convenience. We use the representation in which a given problem has the simpler solution.

4º4. BOX NORMALIZATION:

A box is a system in which potential energy is zero within a closed region and infinite everywhere else. Outside the box, the Schroedinger's equation can be written as:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + \infty \psi = E\psi. \tag{20}$$

This is satisfied only if $\psi=0$ for all points outside the box.

Now, the wavefunction will be well behaved if the wavefunction inside the box joins smoothly with the wavefunction outside of it, for which it must go to zero at the walls of the box. Hence the momentum eigenfunctions cannot exist within a box, since these eigenfunctions do not vanish anywhere. By taking the box to be of arbitrarily large but finite volume, the effect of the presence of the walls can be made negligible apart from the fact that continuous set of eigenvalues are now discrete. We have standing waves in the box; ie., waves of equal amplitude travelling in opposite directions and having wavelengths equal to integral submultiple of 'L', the length of the box. It is usually found convenient to replace the condition $\psi=0$ at the walls by a less stringent one, called the periodic boundary condition. The periodic boundary condition is equivalent to a situation in which the entire infinite space is divided into adjacent cubes and all wavefunctions are periodic throughout the space with the period L, along each of the three axes. Thus along x-axis,

or

$$\psi(x) = \psi(x+L)$$

$$e^{ik_x x} = e^{ik_x (x+L)}$$

$$\Rightarrow e^{ik_x L} = 1.$$

 $\therefore k_x = \pm \frac{2\pi n_x}{L}, \text{ where } n_x \text{ is a positive integer.}$

Similarly, along y and z-axis we have

$$k_y = \pm \frac{2\pi n_y}{L}$$
 and $k_z = \pm \frac{2\pi n_z}{L}$,

 n_y and n_z are positive integers. The spacing of neighbouring k vectors and that of their energy eigenvalues, $\left(\frac{\dot{h}^2k^2}{2m}\right)$, can be made as small as desired by making L sufficiently large.

Thus, if the momentum eigenfunctions obey periodic boundary condition, we can normalize it in the box. For it we have;

$$|N|^2 \int e^{-i\mathbf{k} \cdot \mathbf{r}} \cdot e^{i\mathbf{k} \cdot \mathbf{r}} d^3r = 1$$
entire space

Now the integral of a periodic function over whole of the range is just equal to the integral over only the period of the function. Therefore, we can write the above integral as:

$$|N|^2 \int e^{-i\mathbf{k} \cdot \mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{r}} d^3r = 1$$
cube of vol. L^3

OT

$$|N|^2 L = 1 \Rightarrow N = L^{-3/2}$$

where the arbitrary phase factor of N is taken to be unity for convenience. Hence the normalized momentum eigenfunctions inside a cubical box of side L can be written as:

$$\psi(\mathbf{k}) = \frac{1}{L^{3/2}} e^{i\mathbf{k} \cdot \mathbf{r}}$$
 ...(21)

For the orthonormality of the momentum eigenfunctions we have

$$\int_{-\infty}^{+\infty} \psi^*(\mathbf{k}) \ \psi(\mathbf{k}') \ d^3r$$

because, from the periodicity of the wavefunction, the integrals vanish unless the argument of each exponential is zero. δ 's are the Kronecker deltas. The box is taken to be centred about the origin and hence the limits are from -L/2 to +L/2.

4.5. DIRAC DELTA FUNCTION NORMALIZATION:

We have normalized the momentum eigenfunctions inside a cubical box. We can also use the definition of the delta function to fix the normalization constant of the free-particle momentum eigenfunctions having the form (15) over all space with all real vectors \mathbf{k} . For the discrete spectrum case of the particle in a box, the normalization condition is fixed by the equation (22), where $\delta_{k'}$, k is the Kronecker delta. Analogously, the normalization condition for the continuous spectrum can be written by replacing the Kronecker delta with Dirac delta function. Hence the normalization condition for the free-particle momentum eigenfunction can be written as:

$$\int_{-\infty}^{+\infty} \psi^*(\mathbf{k}) \ \psi(\mathbf{k}') \ d^3r = \delta(\mathbf{k}' - \mathbf{k}) \qquad \dots (23)$$

Using eqn. (15), we can write it as:

$$|N|^{2} \int_{-\infty}^{+\infty} e^{i(\mathbf{k}'-\mathbf{k}) \cdot \mathbf{r}} d^{3}r = \delta(\mathbf{k}'-\mathbf{k})$$

$$|N|^{2} (2\pi)^{3} \delta(\mathbf{k}'-\mathbf{k}) = \delta(\mathbf{k}'-\mathbf{k})$$

$$\Rightarrow N = \frac{1}{(2\pi)^{3/2}},$$

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where the arbitrary phase factor of N is taken to be unity for convenience. Hence the particle momentum eigenfunction, normalized over the entire space, can be written as:

$$\psi(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k} \cdot \mathbf{r}} \qquad ...(24)$$

In terms of the momentum p, the normalization of

$$\psi(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} \qquad \dots (25)$$

is defined by the equation:

$$\int_{-\infty}^{+\infty} \phi^*(\mathbf{p}) \ \phi(\mathbf{p}') \ d^3r = \delta(\mathbf{p}' - \mathbf{p}) \qquad \dots (26)$$

4.6. SCHROEDINGER EQUATION IN MOMENTUM REPRESENTATION:

The Schroedinger equation in the space representation $\psi(\mathbf{r}, t)$ is written as:

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r}) \psi(\mathbf{r}, t) \qquad ...(27)$$

We shall derive the Schroedinger equation in momentum representation $\phi(\mathbf{p}, t)$ from this equation by using equation (9-b), which gives $\phi(\mathbf{p}, t)$ from $\psi(\mathbf{r}, t)$ For it we differentiate (9-b) with respect to t:

$$\frac{\partial \phi(\mathbf{p}, t)}{\partial t} = \frac{1}{(2\pi\hbar)^{3/2}} \int \frac{\partial \psi(\mathbf{r}, t)}{\partial t} e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} d^3r$$
or
$$i\hbar \frac{\partial \phi(\mathbf{p}, t)}{\partial t} = \frac{i\hbar}{(2\pi\hbar)^{3/2}} \int \frac{\partial \psi(\mathbf{r}, t)}{\partial t} e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} d^3r$$
or
$$i\hbar \frac{\partial \phi(\mathbf{p}, t)}{\partial t} = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}, t) d^3r$$

$$\{\text{Using (27)}\} \dots(28)$$

Integrating the first term on the right hand side by parts

$$\frac{1}{(2\pi\hbar)^{3/2}} \cdot \frac{-\hbar^2}{2m} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \nabla^2 \psi(\mathbf{r}, t) d^3r$$

$$= \frac{-\hbar^2}{2m} \frac{1}{(2\pi\hbar)^{3/2}} \iint e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \nabla \psi \int_n ds$$

$$- \frac{\hbar^2}{2m} \cdot \frac{1}{(2\pi\hbar)^{3/2}} \frac{i\mathbf{p}}{\hbar} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \nabla \psi(\mathbf{r}, t) d^3r,$$

where the surface integral over the infinite bounding surface S vanishes, because a wavefunction $\psi \rightarrow 0$ at infinite distances. A second partial integration, in which the surface integral again vanishes, results in:

$$\frac{-\hbar^{2}}{2m} \cdot \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \nabla^{2}\psi(\mathbf{r}, t) d^{3}r$$

$$= \frac{\hbar^{2}}{2m} \cdot \frac{p^{2}}{\hbar^{2}} \cdot \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \psi(\mathbf{r}, t) d^{3}r$$

$$= \frac{p^{2}}{2m} \phi(\mathbf{p}, t) \cdot \dots (29)$$

Using eqns. (29) and 9 (a), we can write (28) as:

$$i\hbar \frac{\partial \phi (\mathbf{p}, t)}{\partial t} = \frac{p^2}{2m} \phi (\mathbf{p}, t) + \frac{1}{(2\pi\hbar)^3} \iint e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} V(\mathbf{r}) e^{i\mathbf{p}'\cdot\mathbf{r}/\hbar} \phi (\mathbf{p}', t) d^3r d^3p' \dots (:0)$$

15.8

Since the potential energy V should be an analytical function of r, we may write

$$e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}V(\mathbf{r}) = V(i\hbar\nabla_{\mathbf{p}})e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \qquad ...(31)$$

Using it, the double integral in (29) can be written as:

Using it, the double integral in (29) can be written as:

$$\frac{1}{(2\pi\hbar)^3} \iint e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} V(\mathbf{r}) e^{i\mathbf{p}' \cdot \mathbf{r}/\hbar} \phi (\mathbf{p}', t) d^3r d^3p'$$

$$= \frac{1}{(2\pi\hbar)^3} \cdot V(i\hbar \nabla_p) \iint e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{r}/\hbar} \phi (\mathbf{p}', t) d^3r d^3p'$$

$$= V(i\hbar \nabla_p) \int \delta (\mathbf{p}' - \mathbf{p}) \phi (\mathbf{p}', t) d^3p'$$

$$= V(i\hbar \nabla_p) \phi (\mathbf{p}, t) \dots (32)$$

Using it in (29) we get:

$$i\hbar \frac{\partial \phi(\mathbf{p}, t)}{\partial t} = \frac{p^2}{2m} \phi(\mathbf{p}, t) + V(i\hbar \nabla_{\mathbf{p}}) \phi(\mathbf{p}, t) \quad ...(33)$$

This is the Schroedinger equation in the momentum representation. This equation is of course, equivalent to (27), the choice between them is only a matter of mathematical convenience.

PROBLEMS

The Gaussian function is represented by $\psi(x) = \frac{1}{\sqrt{\{\sigma\sqrt{(\pi)}\}}}e^{-x^2/2\sigma^2}$

where o is the width of wave packet. Calculate the amplitude function a(k) is given by.

Sol. According to equation (3b), the amplitude function

a(k).

$$a(k) = \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} \psi(x) e^{-ikx} dx$$

$$= \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{\{\sigma\sqrt{(\pi)}\}}} e^{-x^2/2\sigma^2} \cdot e^{-ikx} dx$$

$$= \frac{1}{\sqrt{(2\pi)}} \cdot \frac{1}{\sqrt{\{\sigma\sqrt{(\pi)}\}}} \int_{-\infty}^{+\infty} e^{-(x^2-k^2\sigma^4+2ik\sigma^2x+k^2\sigma^4)/2\sigma^2}$$

$$= \frac{e^{-k^2\sigma^2/2}}{\sqrt{\{2\pi\sigma\sqrt{(\pi)}\}}} \int_{-\infty}^{+\infty} e^{-(x+ik\sigma^2)/2\sigma^2} dx.$$

$$= \frac{e^{-k^2\sigma^2/2}}{\sqrt{\{2\pi\sigma\sqrt{(\pi)}\}}} (x+ik\sigma^2)^2 = u^2 \text{ in the above integral, we have}$$

$$a(k) = \frac{e^{-k^2\sigma^2/2}}{\sqrt{\{2\pi\sigma\sqrt{(\pi)}\}}} \cdot \sqrt{(2)\sigma} \int_{-\infty}^{+} e^{-u^2} du$$

$$= \frac{e^{-k^2\sigma^2/2}}{\sqrt{\{2\pi\sigma\sqrt{(\pi)}\}}} \sqrt{(2)} \sigma \cdot \sqrt{(\pi)} \left\{ : \int_{-\infty}^{+\infty} e^{-u^2} du = \sqrt{(\pi)} \right\}$$

$$\sqrt{\left(\frac{\sigma}{\sqrt{(\pi)}}\right)} e^{-k^2\sigma^2/2}.$$

Problem 2. Find the Fourier transform and the inverse Fourier transform for the function

 $a(k) = \begin{cases} 1/\sqrt{(\epsilon)}, & -\epsilon/2 \leq k \leq \epsilon/2 \\ 0, & |k| > \epsilon/2. \end{cases}$

Show that the inverse Fourier transform is identical to the given function. Also verify the Parseval's formula

Fourier transform of this function is given by:

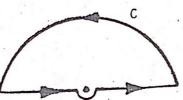
$$\psi(x) = \frac{1}{\sqrt{(2\pi)}} \int_{-\epsilon/2}^{\epsilon/2} \frac{1}{\sqrt{(\epsilon)}} e^{ikx} dk = \sqrt{\left(\frac{2}{\pi\epsilon}\right)} \frac{\sin\left(\frac{\epsilon x}{2}\right)}{x}...(i)$$

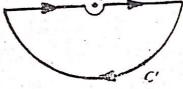
The inverse transform is

and the set transform is
$$a(k) = \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} \frac{\sqrt{2}}{\sqrt{(\pi\epsilon)}} \frac{\sin\left(\frac{\epsilon x}{2}\right)}{x} e^{-ikx} dx$$

$$= \frac{1}{\sqrt{(\epsilon)}} \cdot \frac{1}{2:i} \left[\int_{-\infty}^{+\infty} \frac{e^{i(\epsilon/2-k)x}}{x} dx - \int_{-\infty}^{+\infty} \frac{e^{-i(\epsilon/2+k)x}}{x} dx \right] \dots (ii)$$

Supposing that $-\epsilon/2 \le k \le \epsilon/2$, the exponent in the first integral is positive imaginary, and in the second integral, negative





The path is therefore to be closed in the upper halfplane in the first case, and in the lower half-plane in the second case. The only pole is at Z=0.

a(k) =
$$\frac{1}{\sqrt{(\epsilon)}} \frac{1}{2\pi i} \left[\int_C \frac{e^{i(\epsilon/2-k)z}}{z} dz - \int_C \frac{e^{-i(\epsilon/2+k)z}}{z} dz \right]$$

Using the residue theorem we get:
$$a(k) = \frac{1}{\sqrt{(\epsilon)}} \left\{ \frac{Res}{z=0} \frac{e^{i(\epsilon_1 2 - k)z}}{z} \right\} = \frac{1}{\sqrt{(\epsilon)}} \qquad ...(iii)$$

If $k < -\epsilon/2$, the contours for both integral are to be closed in the upper half-plane, and since the residues for the two integrals are the same, they cancel each other. If $k > \frac{\epsilon}{2}$, the contours are

closed in the lower half-plane, and neither integrand has a singularity within the contour, so that the result is again zero.

Hence in both cases:

oth cases: ...(iv)
$$a(k)=0$$
 for $|k|>\epsilon/2$.

From (iii) and (iv) we see that the inverse Fourier fransform is identical to the given function.

Lastly, to verify the Parseval's formula we have,

$$\int_{-\infty}^{+\infty} |a(k)|^2 dk = \int_{-\epsilon/2}^{\epsilon/2} \frac{1}{\epsilon} dk = 1, \qquad ...(v)$$

and
$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \frac{2}{\pi \epsilon} \int_{-\infty}^{+\infty} \frac{\sin^2\left(\frac{\epsilon x}{2}\right)}{x^2} dx$$
$$= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx \left\{ \text{Replacing} \frac{\epsilon x}{2} \text{ by } x \right\}$$

The value of the above integral can be evaluated by using residue theorem,

$$\int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx = \pi.$$

$$\therefore \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$
...(vi)
$$\therefore \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

From (v) and (vi) we see that the Parseval's formula is satisfied.

Problem 3. The Dirac delta function ' $\delta(x)$ ' has been defined as:

$$\delta(x) = 0 \text{ if } x \neq 0$$

$$\delta(0) = \infty \text{ such that } \int_{-\infty}^{+\infty} \delta(x) dx = 1.$$
 ...(i)

Show that we can also define it alternatively as:

$$\delta(x) = \lim_{g \to \infty} \frac{\sin gx}{\pi x}.$$

We have seen that the difinition (i) is equivalent to the definition,

$$\delta'(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk$$

From it we can write,

$$\delta(x) = \frac{\text{Lim}}{g \to \infty} \frac{1}{2\pi} \int_{-g}^{+g} e^{ikx} dk.$$

$$= \frac{\text{Lim}}{g \to \infty} \frac{1}{2\pi} \frac{2 \sin gx}{x}$$

$$= \frac{\text{Lim}}{g \to \infty} \frac{\sin gx}{\pi x} \qquad \dots \text{(ii)}$$

Problem 4. Show that

$$\frac{d\theta(x),}{dx} = \delta(x),$$

where $\theta(x)$ is the unit step function:

$$\theta(x) = \begin{cases} 1, & \text{for } x > 0 \\ 0, & \text{for } x < 0. \end{cases}$$

Sol. We know that the function $\delta(x)$ satisfies the relation:

$$\int_{-\infty}^{+\infty} f(x) \, \delta(x) \, dx = f(0) \qquad \dots (i)$$

Substituting $\frac{d\theta(x)}{dx}$ for $\delta(x)$ in (i), for two positive numbers

a and b, we find on integrating by parts that

$$\int_{-b}^{a} f(x) \frac{d\theta(x)}{dx} dx = \left[f(x) \dot{\theta}(x) \right]_{-b}^{a} - \int_{-b}^{a} f'(x) \dot{\theta}(x) dx$$

$$= f(a) - \int_{0}^{a} f'(x) dx = f(0) \qquad \dots (ii)$$

Taking a and b as infinite we can see that

$$\frac{d\theta(x)}{dx} = \delta(x)..$$

Problem 5. Prove the following properties of the delta function:

(i)
$$\delta(x) = \delta(-x)$$

(ii)
$$\delta'(x) = -\delta'(-x)$$

(iii)
$$x \delta(x) = 0$$

(iv)
$$x\delta'(x) = -\delta(x)$$
.

$$(v) \qquad \delta(ax) = \frac{1}{a} \delta(x); \ a > 0$$

(vi)
$$\delta(x^2-a^2) = \frac{1}{2a} [\delta(x-a) + \delta(x+a)], a > 0$$

(vii)
$$\int \delta(a-x) \, \delta(x-b) \, dx = \delta(a-b),$$

(viii)
$$f(x) \delta(x-a) = f(a) \delta(x-a)$$
,

Sol. Let us consider a differentiable function f(x), then

(i)
$$\int_{-\infty}^{+\infty} f(x) \, \delta(x) \, dx = f(0)$$

and
$$\int_{-\infty}^{+\infty} f(x) \, \delta(-x) \, dx = \int_{-\infty}^{+\infty} f(-t) \, \delta(t) \, dt = f(0)$$

$$\delta(x) = \delta(-x)$$

(ii)
$$\int_{-\infty}^{+\infty} \delta'(x) f(x) dx = \left[\delta(x) f(x) \right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \delta(x) f'(x) dx$$
 {integrating by parts}

$$= -\int_{-\infty}^{+\infty} \delta(x) f'(x) dx \{ :: f(x) \text{ is differentiable and hence}$$

$$= -f'(0) \qquad \text{vanishes for } \pm \infty \}$$
and
$$\int_{-\infty}^{+\infty} \delta'(-x) f(x) dx = \int_{-\infty}^{+\infty} \delta'(t) f(-t) dt = f'(0)$$

$$\therefore -\delta'(-x) = \delta'(x)$$
(iii)
$$\int_{-\infty}^{+\infty} x \delta(x) f(x) dx = 0, f(0) = 0 \Rightarrow x \delta(x) = 0.$$
(iv)
$$\int_{-\infty}^{+\infty} x \delta(x) f(x) dx = 0, f(0) = 0 \Rightarrow x \delta(x) = 0.$$

(iv)
$$\int_{-\infty}^{+\infty} x \, \delta'(x) f(x) \, dx = -\int_{-\infty}^{+\infty} \delta(x) \left[f(x) + xf'(x) \right] dx$$

(Integrating by parts)

$$= -\int_{-\infty}^{+\infty} f(x) \, \delta(x) \, dx \Rightarrow x \, \delta'(x) = -\delta(x)$$

$$(y) \int_{-\infty}^{+\infty} \delta(ax) \, f(x) \, dx = \frac{1}{2} \int_{-\infty}^{+\infty} \delta(x) \, dx = \frac{$$

(v)
$$\int_{-\infty}^{+\infty} \delta(ax) f(x) dx = \frac{1}{a} \int_{-\infty}^{+\infty} \delta(t) f\left(\frac{t}{a}\right) dt$$
$$= \frac{1}{a} f(0)$$

also,
$$\int_{-\infty}^{+\infty} \frac{1}{a} \delta(x) f(x) dx = \frac{1}{a} f(0).$$

(vi)
$$\int_{-\infty}^{+\infty} f(x) \, \delta(x^2 - a^2) \, dx = \int_{-\infty}^{\infty} f(x) \, \delta(x^2 - a^2) \, dx + \int_{0}^{+\infty} f(x) \, \delta(x^2 - a^2) \, dx. \quad \dots (a)$$

Putting $x^2-a^2=t$ we get $x=\pm\sqrt{(t+a^2)}$ $dx=\pm\frac{1}{2}(t+a^2)^{-1/2} dt$.

We take + ive sign in the second term and negative sign in the first term on the right hand side of (a). We get:

$$\int_{-\infty}^{+\infty} f(x) \, \delta(x^2 - a^2) \, dx = \int_{-a^2}^{+\infty} \frac{f\{-\sqrt{(t+a^2)}\}}{2\sqrt{(t+a^2)}} \, \delta(t) \, dt + \int_{-a^2}^{+\infty} \frac{f\{\sqrt{(t+a^2)}\}}{2\sqrt{(t+a^2)}} \delta(t) \, dt.$$

$$= \frac{f(-a)}{2a} + \frac{f(a)}{2a}. \qquad \dots (b)$$

Also we have:

$$\frac{1}{2a} \int_{-\infty}^{+\infty} f(x) \left[\delta(x-a) + \delta(x+a) \right] dx = \frac{1}{2a} [f(a) + f(-a)]...(c)$$

From (b) and (c), we see that

$$\delta(x^2-a^2) = \frac{1}{2a} [\delta(x-a) + \delta(x+a)],$$

(vii) Multiplying both the sides of the equation by f(a) and integrating over a, we get

L.H.S.=
$$\iint f(a) \, \delta(a-x) \, \delta(x-b) \, dx \, da$$

$$= \int f(x) \, \delta(x-b) \, dx$$

$$= f(b)$$
R.H.S.=
$$\int f(a) \, \delta(a-b) \, da = f(b)$$

$$\therefore \int \delta(a-x) \, \delta(x-b) \, dx = \delta(a-b)$$

(viii) To prove the last identity, we integrate both sides over x, we get

L.H.S.=
$$\int f(x) \, \delta(x-a) \, dx = f(a)$$
and R.H.S.=
$$\int f(a) \, \delta(x-a) \, dx = f(a).$$

$$\therefore f(x) \, \delta(x-a) = f(a) \, \delta(x-a).$$

Problem 7. The lowest energy state of hydrogen atom in the coordinate representation is given by:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{(\pi a_0^3)}} e^{-r/a_0}; \text{ where } a_0 \text{ is a constant.}$$

Find the corresponding momentum representation.

Sol. The momentum representation ϕ (p) is given by the formula:

ula:

$$\phi(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \psi(\mathbf{r}) d^{3}r$$

$$= \frac{1}{(2\hbar)^{3/2}} \cdot \frac{1}{\sqrt{(\pi a_{0}^{3})}} \int e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} e^{-r/a_{0}} r^{2} dr \sin \theta d\theta d\phi.$$
...(i)

In order to evaluate the above integral, we consider an integral of the type,

$$I = \int e^{i\mathbf{k} \cdot \mathbf{r}} f(r) r^2 dr \sin \theta d\theta d\phi$$

$$= 2\pi \int_0^\infty \int_{-1}^{+1} e^{ikr \cos \theta} f(r) r^2 dr d(\cos \theta)$$

$$= 2\pi \int_0^\infty f(r) r^2 dr \frac{e^{ikr} - e^{-ikr}}{ikr}$$

$$= \frac{4\pi}{k} \int_0^\infty \sin kr f(r) r dr. \qquad ...(ii)$$

Using (ii), we can write

$$\phi(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \cdot \frac{1}{\sqrt{(\pi a_0^3)}} \cdot \frac{4\pi}{(-p/\hbar)} \cdot \int_0^\infty \sin\left(-\frac{pr}{\hbar}\right) e^{-r/a_0} dr$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} \cdot \frac{1}{\sqrt{(\pi a_0^3)}} \cdot \frac{4\pi\hbar}{p} \int_0^\infty \sin\left(\frac{pr}{\hbar}\right) e^{-r/a_0} r dr \dots (iii)$$

Now.

$$\int_{0}^{\infty} \sin\left(\frac{pr}{\hbar}\right) e^{-r/a_{0}} r dr = I_{m}. \int_{0}^{\infty} e^{-r(1/a_{0} - ip/\hbar)} r dr$$

$$= I_{m}. \frac{1}{\left(\frac{1}{a_{0}} - \frac{ip}{\hbar}\right)^{2}} \left\{ \text{Using } \int_{0}^{\infty} r^{n} e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}} \right\}$$

$$= \frac{2\frac{p}{\hbar}.\frac{1}{a_{0}}}{\left(\frac{1}{a_{0}^{2}} + \frac{p^{2}}{\hbar^{2}}\right)^{2}}.$$

$$\Rightarrow \phi(\mathbf{p}) = \frac{1}{\pi} \left(\frac{2a_{0}}{\hbar}\right)^{n/2} \frac{\hbar^{4}}{(\hbar^{2} + p^{2}a_{0}^{2})^{2}}.$$

Remarks. To find the dimensions of ϕ (p), we note that \hbar has the dimensions of energy \times time $=ML^2T^{-1}$, a_0 has the dimension of length and p is momentum with dimension MLT^{-1} . Hence the dimensions of ϕ (p) can be seen to be $\frac{1}{(MLT^{-1})^{3/2}}$, i.e. that of $p^{-3/2}$. From this dimensions of ϕ (p) we see that the quantity $\phi^*\phi$ d^3p , the probability in the momentum space, comes out to be dimensionless as it should be.

Problem 8. Change the function,

$$\phi(p_x) = exp \left\{ -i \left(\frac{p_x^3}{6m} - E_p \right) \right/ \hbar \right\},$$

to the coordinate representation.

Sol. The wavefunction in the coordinate representation is given by

$$\psi(x) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} \phi(p_x) \exp\left\{ip_x x/\hbar\right\} dp_x$$

$$= \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} \exp\left\{-i\left(\frac{|p_x|^3}{6m} - E_p\right)/\hbar\right\} \exp\left\{ip_x x/\hbar\right\} dp_x.$$

Changing the variable of integration to $u=-(2m\hbar)^{-1/3} p_x$, we obtain,

$$\psi(x) = \frac{\alpha}{\sqrt{(2\pi)}} \int_{-\infty}^{+\infty} e^{i(u^3/3) - iuy} du = \frac{\sqrt{(2)} \cdot \alpha}{\sqrt{(\pi)}} \int_{0}^{\infty} \cos\left(\frac{u^3}{3} - uy\right) du,$$
where, $\alpha = (2m\hbar^{\frac{1}{2}/2})^{1/3}$ and $y = (x + E_p) \alpha$.

Problem 9. Express the operator $\frac{1}{p}$ in the coordinate representation, and the operator $\frac{1}{x}$ in momentum representation, for motion

in one dimension.

Sol. Let us denote by $\psi'(x)$ the result of the operation $\frac{1}{p}$ on $\psi(x)$, i.e.

$$\frac{1}{p} \psi(x) = \psi'(x). \qquad \dots (i)$$

If $\phi(p)$ and $\phi'(p)$ are the Fourier transforms of $\psi(x)$ and $\psi'(x)$; respectively, equation (i) can be written as

$$\frac{1}{p} \phi(p) = \phi'(p). \qquad \dots (ii)$$

This equation shows that $\phi'(p)$ has a pole at p=0, and thus does not in general have the properties of continuity etc., which must be satisfied by the wavefunction. In order to avoid this, it is necessary that $\phi(0)=0$, which in coordinate representation becomes

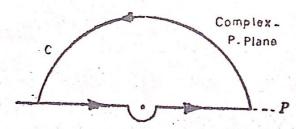
$$\int_{-\infty}^{+\infty} \psi(x) dx = 0. \qquad ...(iii)$$

From (i) and (ii), we have

$$\psi'(x) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} \frac{\phi(p)}{p} e^{ipx/\hbar} dp. \qquad ...(iv)$$

By choosing the contour of integration as shown below, we can write

$$\psi'(x) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_C \frac{\phi(p)}{p} e^{ipx/\hbar} dp. \qquad ...(v)$$



Now, by definition,

$$\phi(p) = \frac{1}{\sqrt{(2\pi\hbar)}} \int_{-\infty}^{+\infty} \psi(x') e^{-ipx'/\hbar} dx'. \qquad ...(vi)$$

Substituting (vi) in (v), we obtain

$$\psi'(x) = \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} \psi(x') dx' \int_{C} \frac{\exp\{-ip(x-x')/\hbar\}}{p} dp. \dots (vii)$$
Evaluating the second integral in the second in the

Evaluating the second integral by the residue method, we find that

$$\int_{C} \frac{\exp\left\{-ip (x-x')/\hbar\right\}}{p} dp = \begin{cases} 2\pi i & \text{if } x > x' \\ 0 & \text{if } x < x'. \end{cases}$$

Putting this value in (vii), we have

$$\psi'(x) = \frac{i}{\hbar} \int_{-\infty}^{\infty} dx' \, \psi(x'). \qquad \dots \text{(viii)}$$

Comparing with (i),

$$\frac{1}{p} = \frac{i}{\hbar} \int_{-\infty}^{x} dx'.$$
 ...(ix)

For the operator $\frac{1}{x}$ in the momentum representation, we obtain similarly the relation

$$\frac{1}{x} = \frac{1}{i\hbar} \int_{-\infty}^{p'} dp'. \qquad \dots (x)$$

Problem 10. Show that the transformation from the position diagonal representation to the momentum diagonal representation is unitary.

Solution. The transformation from the coordinate representation to the momentum representation is given by the Fourier transform. If ψ (r) is the wavefunction in the coordinate representation, then the wavefunction ϕ (p) in the momentum representation is given by

$$\phi$$
 (p) = $\frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \psi$ (r) d^3r ...(i)

Thus, by the operation of the integral operator,

$$U = \frac{1}{(2\pi\hbar)^{3/2}} \int d^2r \ e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} \qquad \dots (ii)$$

on the position representation we can obtain the momentum representation.

In the position representation, r becomes a diagonal matrix with the elements,

$$\mathbf{r}_{\mathbf{r}, \mathbf{r}'} = \mathbf{r} \delta (\mathbf{r} - \mathbf{r}')$$
 .. (iii)

In the position representation, $\mathbf{p} = -t \mathbf{\hat{n}} \nabla$ is an off-diagonal matrix with the elements

$$\mathbf{p}_{\mathbf{r}, \mathbf{r}'} = -i\hbar \nabla \delta (\mathbf{r} - \mathbf{r}')$$
 ...(iv)

While, it is a diagonal matrix in the momentum representation with the elements:

$$\mathbf{p}_{\mathbf{p}, \mathbf{p}'} = \mathbf{p} \, \delta \, (\mathbf{p} - \mathbf{p}') \qquad \dots (\mathbf{v})$$

We can go to the momentum representation (in which p is diagonal) from the position representation by a unitary transformation with U as:

on with
$$U$$
 as:
$$U^{\dagger} p_{\mathbf{p}, \mathbf{p}'} U = \frac{1}{(2\pi\hbar)^3} \iint e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} \left[-i\hbar \nabla \delta \left(\mathbf{r} - \mathbf{r}' \right) \right]$$

$$= \frac{-i\mathbf{p}' \cdot \mathbf{r}'/\hbar}{d^3 r} \frac{d^3 r}{d^3 r}$$

$$= \frac{1}{(2\pi\hbar)^3} \int e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} \left[-i\hbar \nabla \right] e^{-i\mathbf{p}' \cdot \mathbf{r}/\hbar} d^3 r$$

$$= \mathbf{p}' \frac{1}{(2\pi\hbar)^3} \int e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} e^{-i\mathbf{p}' \cdot \mathbf{r}/\hbar} d^3 r$$

$$= \mathbf{p}' \delta \left(\mathbf{p} - \mathbf{p}' \right) = \mathbf{p} \delta \left(\mathbf{p} - \mathbf{p}' \right)$$

Thus, the transformation from position diagonal representation to momentum diagonal representation is unitary, where the transformation matrix is the continuous matrix *U*, given by eq. (ii).

SOME SIMPLE APPLICATIONS OF THE SCHROEDINGER EQUATION

In order to get an insight into the methods of quantum mechanics, in this chapter, we shall discuss some of the very simple systems which yield exact solutions of the Schroedinger equation. The simplest system is one in which the potential energy of a particle depends on only one coordinate, say x, or a system in which the potential energy can be expressed as a sum of function of single coordinate, $V(\mathbf{r}) = V_1(x) + V_2(y) + V_3(z)$. In the later case we can decompose the Schroedinger equation into a set of three one dimensional equations. Although these systems are only the idealization of the naturally occurring systems, the qualitative features of many physical problems can often be approximated very well by these. For example, the nuclear forces are

not known accurately, it is known that these forces have a short range; they extend to some distance, and then drop to zero very fast. The qualitative features of these forces can be studied by approximating them by a potential of the form shown in the adjacent figure (1) frequently called a square well potential.

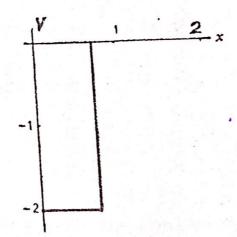


Fig. 1. Square well Potential

5.1. THE FREE PARTICLE:

A free particle is one whose potential energy is independent of

the position. Conveniently it is chosen to be zero. Then the Schroedinger equation for one dimensional motion of the free particle can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=E\psi(x)$$

 $\{:: V=0 \text{ for the free particle}\}$

or
$$\frac{d^2 \psi(x)}{ax^2} + \alpha^2 \psi(x) = 0, \text{ where } \alpha = \sqrt{\left(\frac{2mE}{\hbar^2}\right)}. \dots (1)$$

It is a second order linear differential equation and has a general solution of the form

$$\psi(x) = Ae^{i\alpha x} + Be^{-i\alpha x}, \qquad \dots (2)$$

where A and B are constants. Since there are no boundary conditions to be satisfied, all the constants, including a, can have any value we want to give them. Therefore, the particle moves with continuous energy eigenvalues.

Now we consider the Schroedinger equation for the three dimensional motion of a free particle:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi$$
or
$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2mE}{\hbar^2} \psi = 0. \qquad ...(3)$$

We can solve this equation by the method of separation of We write \u00fc as the product of three independent funcvariables. tions as:

$$\psi = X(x) Y(y) Z(z). \qquad ...(4)$$

Substituting this in equation (3) and dividing by X(x), Y(y), Z(z), we get

$$\frac{1}{X} \frac{\partial^{2}X}{\partial x^{2}} + \frac{1}{Y} \frac{\partial^{2}Y}{\partial y^{2}} + \frac{1}{Z} \frac{\partial^{2}Z}{\partial z^{2}} + \frac{2mE}{\hbar^{2}} = 0$$
or
$$\frac{1}{X} \frac{\partial^{2}X}{\partial x^{2}} = -\frac{1}{Y} \frac{\partial^{2}Y}{\partial y^{2}} - \frac{1}{Z} \frac{\partial^{2}Z}{\partial z^{2}} - \frac{2mE}{\hbar^{2}}. \qquad .. (5)$$

Left hand side of the above equation is a function of x only while the right hand side does not depend on x. Hence the differentiation of the left hand side w.r t. x should be zero. Therefore, each side of (5) should be equal to the same constant, say $-k_x^2$,

then
$$\frac{1}{X} \frac{\partial^2 X}{\partial x^2} = -k_x^2 \qquad ...(6)$$
 and
$$-\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} = -k_x^2$$
 or
$$\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} = k_x^2 - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} \qquad ...(7)$$

In (7) left hand side is a function of only y while right hand side does not involve y. So each side will be equal to some tant $-k_{\nu}^{2}$ (say) so that

or

$$\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} = -k_{y^2} \qquad \dots (8)$$

and

$$k_x^2 - \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} - \frac{2mE}{\hbar^2} = -k_y^2$$

or

$$\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = k_x^2 + k_y^2 - \frac{2mE}{\hbar^2}.$$
 ...(9)

The right hand side of the above equation is a constant. Let us denote it by $-k_z^2$, so that we may write

$$\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = -k_z^2 \qquad \dots (10)$$

and

$$k_x^2 + k_y^2 - \frac{2mE}{\hbar^2} = -k_z^2$$

or

$$E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2). \tag{11}$$

Taking k_x , k_y and k_z as the components of a vector \mathbf{k} , known as the propagation vector, we have

$$E = \frac{\hbar^2 k^2}{2m} \qquad \dots (12)$$

Now the solution of equation (6) is given by,

$$X(x) = e^{\pm ik_x x} \qquad \dots (13)$$

Solution e^{ik_xx} represents a wave travelling in the positive x-direction while e^{-ik_xx} represents a wave moving in the negative x-direction. Taking the propagation vector as negative for a wave travelling in the negative direction, we can write the solution as:

Similarly, the solutions of (8) and (10) are given by,

and

$$Z(z) = e^{ik_z z} \qquad \dots (16)$$

Hence the solution ' ψ ' of equation (3) is given by,

$$\psi = e^{i(k_x x + k_y y + k_z z)} = e^{i\mathbf{k} \cdot \mathbf{r}} \qquad \dots (17)$$

This is known as a plane wave. Since there are no boundary conditions to be satisfied by the solution (17), k_x , k_y and k_z can have all real values and hence the energy eigenvalues of the free particle form a continuous set.

5.2. PARTICLE IN A ONE DIMENSIONAL BOX:

In quantum mechanics, a box means a system in which the potential energy is zero within a closed region and infinite everywhere else. For one dimensional box of length a, therefore,

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a \\ \infty & \text{for } x < 0 \text{ and } x > a \end{cases} \dots (18)$$

Outside the box the wave equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \cos\psi = E\psi. \tag{19}$$

It can be satisfied only if $\psi=0$ at all points outside the box.

Inside the box, wave equation is given by eqn. (1) and the solution can be written as

$$\psi(x) = Ae^{i\alpha x} + Be^{-i\alpha x}.$$
 (20)

Now ψ has to satisfy boundary conditions at x=0 and x=a. From the continuity of the solution at x=0 and x=a, we have

$$A+B=0 \qquad \dots (21)$$

and

$$Ae^{i\alpha a} + Be^{-i\alpha a} = 0 \qquad \dots (22)$$

From (21) we have B = -A and hence (22) gives

$$A (e^{i\alpha_a} - e^{-i\alpha_a}) = 0$$

2*iA* sin $\alpha a = 0$

or

$$\Rightarrow \sin \alpha a = 0 \Rightarrow \alpha a = n\pi \; ; \; n = 1, 2, 3, \dots \qquad \dots (23)$$

Here A cannot be zero because in that case B = -A will also be zero and hence the solution (20) will vanish. Thus the solution (20) can be written as:

written as:

$$\psi(x) = A \left(e^{i\alpha ax} - e^{-i\alpha x} \right) = 2iA \sin \alpha x$$

$$= C \sin \alpha x,$$

$$= C \sin \alpha x,$$

$$= C \sin \alpha x,$$

where C=2iA is another constant. Choosing C to normalize ψ , we have

$$|C|^{2} \int_{0}^{a} \sin^{2} \alpha x \, dx = 1$$

$$|C|^{2} \int_{0}^{a} \sin^{2} \frac{n\pi}{a} x \, dx = 1$$
 [Using (23)]

or

$$|C| \int_0^a dx dx$$

$$|C|^2 \frac{a}{2} = 1 \Rightarrow C = \sqrt{\left(\frac{2}{a}\right)}$$

or

Hence the normalized wavefunction is given by,

$$\psi(x) = \sqrt{\left(\frac{2}{a}\right)} \sin \alpha x. \qquad \dots (25)$$

To find the energy eigenvalues, we have from eqn. (23), that $\alpha^2 a^2 = n^2 \pi^2$

Alka

or
$$\frac{2mE}{\hbar^2} a^2 = n^2 \pi^2 \left(: \alpha = \sqrt{\left\{ \frac{2mE}{\hbar^2} \right\}} \right)$$

$$\Rightarrow E = \frac{\pi^2 \hbar^2 n^2}{2ma^2}, n = 1, 2, 3, \dots \tag{26}$$

Thus the energy of the particle in a box is consisted of a set of discrete values corresponding to different values of n. In general, whenever there is some boundary condition to be satisfied, the eigenvalue spectrum will come out to be discrete. For free particles the spectrum is continuous. For a particle in a box if we let $a \rightarrow \infty$, then the spacing between energy levels approaches zero, and so the spectrum approaches a continuous distribution of values. We can regard a continuous spectrum as the limit of discrete spectrum in which the box is allowed to grow to infinite size.

53. PARTICLE IN A THREE DIMENSIONAL BOX:

Let us consider a particle enclosed in a rectangular box of sides a, b and c; respectively, with impenetrable walls, inside which it can move freely. The potential energy can be written in the form, $V(\mathbf{r}) = V_1(x) + V_2(y) + V_3(z)$, where

$$V_1(x) = V_2(y) = V_3(z) = \begin{cases} 0 & \text{if } 0 < x < a, 0 < y < b, 0 < z < c, \\ \infty & \text{outside these intervals.} \end{cases}$$
 ...(27)

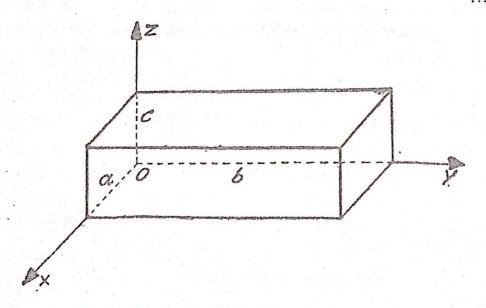


Fig. 2. Three dimensional box of sides a, b and c.

The Schroedinger equation outside the box can be satisfied only if $\psi=0$ at all points outside the box.

Inside the box, the wave-equation is given by eqn. (3) and can be decomposed into three one-dimensional equations as:

13

$$\frac{\partial^{2}X}{\partial x^{2}} + k_{x}^{2}X = 0 ;$$

$$\frac{\partial^{2}Y}{\partial y^{2}} + k_{y}^{2}Y = 0 ;$$
and
$$\frac{\partial^{2}Z}{\partial z^{2}} + k_{z}^{2}Z = 0. \qquad ...(28)$$
Here,
$$k_{x}^{2} + k_{y}^{2} + k_{z}^{2} = \frac{2mE}{\hbar^{2}}. \qquad ...(29)$$

The normalized solution of the first of eqns. (28) can be found exactly in the same way as for the case of one dimensional box. We get.

get.

$$X(x) = \sqrt{\left(\frac{2}{a}\right)} \sin k_x x$$
, with $k_x a = n_x \pi$; $n_x = 1, 2, 3, ...$

Similarly,

Similarly,

$$Y(y) = \sqrt{\left(\frac{2}{b}\right)} \sin k_y y \; ; \; k_y b = n_y \; \pi \; ; \; n_y = 1, \; 2, \; 3, \; \dots$$

and

03

$$Z(z) = \sqrt{\left(\frac{2}{c}\right)} \sin k_z z$$
; $k_z c = n_z \pi$, $n_z = 1, 2, 3, ...$

Hence the normalized solution of the Schroedinger equation for a particle in a box of sides a, b and c is given by:

$$\psi = X(x) \ Y(y) . Z(z).$$

$$= \sqrt{\left(\frac{2}{a}\right)} \sin \frac{n_x \pi}{a} x . \sqrt{\left(\frac{2}{b}\right)} \sin \frac{n_y \pi}{b} y . \sqrt{\left(\frac{2}{c}\right)} \sin \frac{n_z \pi}{c} z$$

$$= \sqrt{\left(\frac{8}{abc}\right)} \sin \frac{n_x \pi}{a} x . \sin \frac{n_y \pi}{b} y . \sin \frac{n_z \pi}{c} z ...(30)$$

The possible values of the energy is given by (29) as:

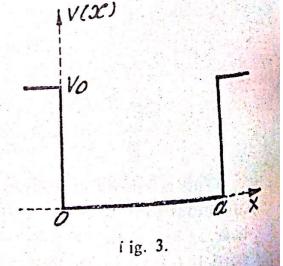
$$E = \frac{\hbar^2 n^2}{2m} \left(\frac{n_x^2}{\sigma^2} + \frac{n_y^2}{\hbar^2} + \frac{n_z^2}{c^2} \right); \quad n_x, n_y, n_z = 1, 2, 3, \dots$$
 ...(31)

PARTICLE IN ONE DIMENSIONAL WELL:

A one dimensional well of depth V_0 , defined by

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a \\ V_0 & \text{for } x < 0 \text{ and } x > a \\ \dots & (32) \end{cases}$$

is shown in figure 3.



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The Schroedinger equation can be written as:

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0, \quad k_1 = \sqrt{\left(\frac{2mE}{\hbar^2}\right)} \ (0 < x < a) \qquad \dots(33-a)$$

$$\frac{d^2\psi}{dx^2} - k_2^2 \psi = 0, \quad k_2 = \sqrt{\left(\frac{2m (V_0 - E)}{\hbar^2}\right)} (x < 0 \text{ and } x > a)$$
...(33-b)

General solution of (33-a) can be found immediately to be: $\psi = A \cos k_1 x + B \sin k_1 x$ (0 < x < a)

The general solution of (33-b) for $E < V_0$ (bound states) can be written immediately as:

$$\psi = Ce^{k_2x} + De^{-k_2x}$$
 (x < 0 and x > a)

where, A, B, C and D are integration constants.

Now the wavefunction ψ should vanish for very large values of $x (x \to \pm \infty)$. The function $e^{k_2 x}$, however, is not bounded as x becomes large and positive; hence, it must not appear in ψ for Similarly, ψ must not contain e^{-k_2x} for x < 0. Hence we have

$$\psi = \begin{cases} Ce^{k_2 x} & (x < 0) \\ De^{-k_2 x} & (x > a) \end{cases} \dots (34-b)$$

It has been pointed out in the last chapter that the wave function and its derivative must be continuous everywhere. potential V(x) is discontinuous at x=0 and x=a in the present problem, the form of the Schroedinger equation changes discontinuously at x=0 and x=a. The continuity of ψ and $\frac{d\psi}{dx}$ at x=0and x=a requires that the constants of integration should be such that:

$$A = C$$
 ...(35-a) ...(35-b)

$$A = C$$

$$-k_2 a \qquad \dots (35-b)$$

$$A\cos k_1 a + B\sin k_1 a = De^{-k_2 a} \qquad ...(35-b)$$

$$L B = k C \qquad ...(35-c)$$

$$k_1 B = k_2 C$$

 $-k_1 A \sin k_1 a + k_1 B \cos k_1 a = -k_2 D e^{-k_2 a}$...(35-d)

From (35-a) and (35-c) we have A=C and $B=\frac{k_2}{k_1}C$.

Putting these values of A and B in (35-b) and (35-d) we obtain:

$$C\left(\cos k_1 a + \frac{k_2}{k_1} \sin k_1 a\right) = De^{-k_2 a}$$
 ...(36-a)

and $C(-k_1 \sin k_1 a + k_2 \cos k_1 a) = -k_2 De^{-k_2 a}$ Dividing (36-a) by (36-b) we get:

or
$$\frac{-k_{1} \sin k_{1}a + \frac{k_{2}}{k_{1}} \sin k_{1} a}{-k_{1} \sin k_{1}a + k_{2} \cos k_{1}a} = \frac{-1}{k_{2}}$$
or
$$k_{1}k_{2} \cos k_{1}a + k_{2}^{2} \sin k_{1}a = k_{1}^{2} \sin k_{1}a - k_{1}k_{2} \cos k_{1}a$$
or
$$(k_{1}^{2} - k_{2}^{2}) \sin k_{1}a = 2k_{1}k_{2} \cos k_{1}a$$

$$\Rightarrow 2 \cot k_{1}a = \frac{k_{1}^{2} - k_{2}^{2}}{k_{1}k_{2}} = \frac{k_{1}}{k_{2}} - \frac{k_{2}}{k_{1}} \qquad ...(37)$$
Introducing the second of the size of the second of the

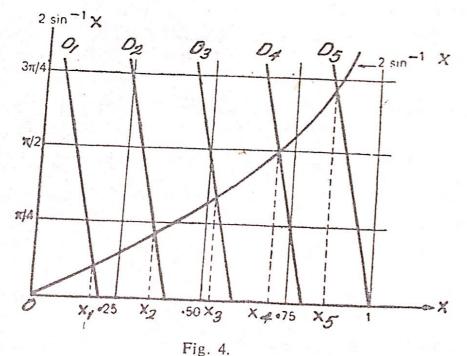
Introducing the quant

$$\gamma = \sqrt{\left(\frac{2mV_0}{\hbar^2}\right)}$$
 and $x = \frac{k_1}{\gamma} = \sqrt{\left(\frac{E}{V_0}\right)}$, ...(38)

we obtain the following transcendental equation:

$$n\pi - a\gamma x = 2 \sin^{-1} x$$
; $n = 1, 2, 3, ...$...(39)

Here $\sin^{-1} x$ is to be taken in the interval $\left(0, \frac{\pi}{2}\right)$. The roots of equation (39) give the energy levels $E = V_0 x^2$. When E increases from 0 to V_0 , x increases from 0 to 1, the right-hand side of equation (39) increases from 0 to π , and the left-hand side decreases from $n\pi$ to $n\pi - a\gamma$ Equation (39) can be solved graphically, by determining the abscissae of the inter-sections of the curve $2 \sin^{-1} x$ with the straight lines $D_n = n \pi - a\gamma x$, figure 4.



The necessary and sufficient condition for at least one of the straight lines D_n to intersect the curve $2 \sin^{-1} x^n$ is that

$$n\pi - a\gamma \leqslant \pi$$
, i.e., $a\gamma \geqslant (n-1)\pi$(40)

Clearly, the condition (40) is satisfied a least for n=1. Hence we see that there always exists a bound state. If $0 \le a\gamma < \pi$ there is one eigenvalue E_1 , and if $\pi \le a\gamma \le 2\pi$ there are two eigenvalues E_1 and E_2 ($E_1 < E_2$), and so on. Thus the energy eigenvalues of a particle in a square well potential constitute a discrete spectrum for the bound states ($E < V_0$). Since V_0 is finite and there cannot be a root greater than $E = V_0$, there will be only a finite number of discrete energy eigenvalues. For $E > V_0$ we have a continuous spectrum.

It should be noted that the particle in a one dimensional box can be considered as a special cass of the particle in a well with infinite depth *i.e.* by taking $V_0 \to \infty$. Then $k_2 \to \infty$. Hence we have from (37) that:

$$\cot k_1 a \to \infty$$

$$\therefore k_1 a = n\pi, n = 1, 2, 3, \dots$$

The characteristic energy values are

$$E = \frac{\pi^2 \hbar^2 n^2}{2ma^2}, n=1, 2, 3, \dots$$

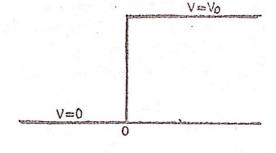
5.5. SQUARE POTENTIAL STEP BARRIER:

The potential step is reprelented by the function

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases} \dots (4)$$

- This is shown in Fig. 5.

The Schroedinger's equation can be written as:



$$\frac{d^2\psi}{dx^2} + k_1^2 \ \psi = 0; \ k_1 = \sqrt{\left(\frac{2mE}{\hbar^2}\right)} \ (x < 0)$$
 Fig. 5 ... (22a)

$$\frac{d^2\psi}{dx^2} + k_2^2 \psi = 0; \ k_2 = \sqrt{\left(\frac{2m (E - V_0)}{\hbar^2}\right)} (x > 0) \qquad \dots (42b)$$

General solutions of eqns. (42) can be found immediately to be:

$$\psi = Ae^{ik_1x} + Be^{-ik_1x} \quad (x < 0) \qquad ...(43a)$$

$$\psi = Ce^{ik_2x} + De^{-ik_2x} (x > 0) \qquad ...(43b)$$

where A, B, C, D are the constants of integration.

In eqn. (43a) the term e^{ik_1x} represents a wave advancing in the positive x-direction; i.e., incident wave, and e^{-ik_1x} represents

a wave moving in the negative direction of x; i.e., reflected wave. In eqn. (43b) the term e^{ik_2x} represents a wave moving in the positive x-direction; i.e., transmitted wave, and e^{-ik_2x} represents a wave moving in the negative x-direction, i.e. reflected wave. Since there is no barrier after x=0 on the right hand side, hence there should not at all arise a question of reflection in this region. Hence the term e^{-ik_2x} should be absent in (43b) and

$$\psi = Ce^{ik_2x} (x > 0) \qquad \dots (43c)$$

As in the last problem, applying the boundary conditions on the solution ψ , which requires that ψ and $\frac{d\psi}{dx}$ should be continuous at x=0, we get:

$$A+B=C$$

$$ik_1 (A-B)=ik_2C$$

From these equations we have

$$C = \frac{2k_1}{k_1 + k_2} A$$

$$B = \frac{k_1 - k_2}{k_1 + k_2} A$$
...(44)

Now we distinguish the following three cases:

(I) $E > V_0$. In this case both of k_1 and k_2 will be real and positive. The incident wave is given by,

$$\psi_{incident} = Ae^{ik_1x}$$

and hence the probability current for incident wave is given as:

$$S_{I} = Re \cdot \left[\frac{\hbar}{im} \psi^{*}_{incident} \frac{\partial \psi_{incident}}{\epsilon x} \right]$$

$$= Re \cdot \left[\frac{\hbar}{im} A^{*}e^{-ik_{1}x} \cdot ik_{1} Ae^{ik_{1}x} \right]$$

$$= \frac{\hbar k_{1}}{m} |A|^{2} \qquad ...(45a)$$

The reflected wave is Be^{-ik_1x} and, therefore, the reflected current is given by

$$S_{R} = \frac{-\ln k_{1}}{m} |B|^{2} = \frac{-\ln k_{1} (k_{1} - k_{2})^{2}}{m (k_{1} + k_{2})^{2}} |A|^{2}. \qquad ...(45b)$$

The transmitted wave is Ce^{ik_2x} and hence the probability current for the transmitted wave is:

$$S_T = \frac{\hbar k_2}{m} |C|^2 = \frac{\hbar k_2}{m} \cdot \frac{4k_1^2}{(k_1 + k_2)^2} |A|^2 \qquad ...(45c)$$

The coefficient of reflection 'R' and the coefficient of transmis sion 'T' are defined as:

$$R = \frac{\text{Magnitude of reflected current}}{\text{Magnitude of incident current}} = \frac{|S_R|}{|S_I|}$$

and

$$T = \frac{\text{Magnitude of transmitted current}}{\text{Magnitude of incident current}} = \frac{|S_T|}{|S_I|}.$$

Hence for this case we have from eqns. (45) that:

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \qquad \dots (46a)$$

and

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \dots (46b)$$

According to definition the sum of reflectance and transmittance must be equal to unity. It can atonce be seen from equations (46) that R+T=1. We can also see from (46) that $R \to 0$ as $k_2 \to k_1$ and $R \to 1$ as $k_2 \to 0$. Now k_2 will approach k_1 if $V_0 = 0$. Hence there must be some reflectance even if $E >> V_0$. This property of reflection from a sudden change in potential arises from wave nature and does not exist in classical theory if $E > V_0$. It is purely a quantum mechanical effect.

(II). $0 < E < V_0$. Here k_1 will be real, while k_2 will be purely imaginary. We write

$$k_2 = i \sqrt{\left(\frac{2m'(V_0 - E)}{\hbar^2}\right)} = ik_2' \text{ (say); } k_2' \text{ is real}$$

Thus the transmitted wave can be written as:

$$\psi_{trans} = Ce^{ik_2x} = Ce^{-k'_2x}$$

Hence the probability current for the transmitted wave will be

$$S_{T} = Re \cdot \left[\frac{\hbar}{im} \psi^{*}_{trans} \cdot \frac{\partial \psi_{trans}}{\partial x} \right]$$

$$= Re \cdot \left[\frac{\hbar}{im} \cdot C^{*}e^{-k'_{2}x} \cdot C(-k'_{2}) e^{-k'_{2}x} \right] = 0$$

$$\therefore T = \left| \frac{S_{T}}{S_{I}} \right| = 0 \qquad ...(47a)$$

Also, the reflected current S_R in this case is given by,

$$S_{R} = \frac{-\ln k_{1}}{m} \frac{|k_{1} - ik'_{2}|^{2}}{|k_{1} + ik'_{2}|^{2}} |A|^{2} = \frac{-\ln k_{1}}{m} |A|^{2}$$

$$\therefore R = \frac{|S_R|}{|S_I|} = 1 \qquad \dots (47b)$$

Thus the incident wave is completely reflected from the step. However, the wavefunction is not zero to the right of the step and has the value Ce^{-k_2x} . Hence, there is a finite probability that the particle is found in a region which is classically inaccessible. This phenomenon of barrier penetration is purely a quantum mechanical effect.

(III) E < 0. The numbers k_1 and k_2 will both the purely imaginary and there is no solution possible in this case.

5.6. RECTANGULAR POTENTIAL BARRIER:

Let us consider the one dimensional motion of a particle under a rectangular potential barrier represented by the function,

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 < x < 0 \\ 0 & \text{for } x > a \end{cases}, \tag{48}$$

shown in fig. 6.

The Schroedinger's equation can be written as:

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0;$$

$$k_{1} = \sqrt{\left(\frac{2mE}{\hbar}\right)} (x < 0) \quad ...(49a)$$

$$\frac{d^{2}\psi}{dx^{2}} - k_{2}{}^{2}\psi = 0;$$

$$k_{2} = \sqrt{\frac{2m(V_{0} - E)}{\hbar^{2}}} (0 < x < a)$$
...(49b)

and $\frac{d^2\psi}{dx^2} + k_1'\psi = 0$;

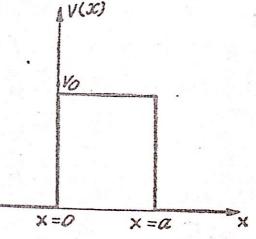


Fig. 6

$$k_1 = \sqrt{\left(\frac{2mE}{\hbar^2}\right)} \quad (x > a) \qquad \dots (49c)$$

General solutions of eqns. (49) can be found immediately to be

$$\psi = Ae^{ik_1x} + Be^{-ik_1x} \qquad (x < 0), \qquad ...(50a)$$

$$\psi = Ce^{k_2 x} + De^{-k_2 x} \qquad (0 \langle x \langle a \rangle \dots (50b))$$

 $\psi = Ce^{k_{2}x} + De^{-k_{2}x} \qquad (0 < x < a) \qquad ...(50b)$ $\psi = Fe^{ik_{1}x} + Ge^{-ik_{1}x} \qquad (x > a) \qquad ...(50c)$ and where A, B, C, D, F and G are constant of integration.

In eqn (50a) first term represents a wave advancing in the positive x-axis direction; i.e., incident wave, and the second term represents a wave moving in the negative direction of x-axis; i.e., reflected wave. Similarly, in eqn. (50b) first term represents a wave transmitted at x=0 and second term represents a wave reflected at x=a. In quation (50c), first term represents a wave transmitted at x=a and the second term represents a wave moving in the negative x-direction. Since there is no obstacle after x=a on the right hand side, there should not at all arise a question of reflection in this region. Hence the second term should be absent in (50c) and

$$\psi = Fe^{ik_1 x}(x > a) \qquad \dots (50 d)$$

Applying the boundary conditions on ψ , which requires that ψ and $\frac{d\psi}{dx}$ should be continuous at x=0 and x=a, we get;

$$A+B=C+D$$
 ...(i)

$$ik_1(A-B) = k_2(C-D)$$
 ...(ii)

$$Ce^{k_{2}a} + De^{-k_{2}a} = Fe^{ik_{1}a} \qquad ...(iii)$$

$$k_2 \left(Ce^{k_2 a} - De^{-k_2 a} \right) = ik_1 Fe^{ik_1 a}.$$
 ...(iv)

From (i) and (ii), we have

$$A = \left(1 + \frac{k_2}{i \, k_1}\right) \frac{C}{2} + \left(1 - \frac{k_2}{i \, k_1}\right) \frac{D}{2} \qquad \dots (v)$$

$$B = \left(1 - \frac{k_2}{i k_1}\right) \frac{C}{2} + \left(1 + \frac{k_2}{i k_1}\right) \frac{D}{2} \qquad \dots \text{(vi)}$$

From (iii) and (iv) we have

$$\hat{C} = \left(1 + \frac{ik_1}{k_2}\right) \frac{F}{2} e^{ik_1 a} e^{-k_2 a} \qquad ...(vii)$$

$$D = \left(1 - \frac{ik_1}{k_2}\right) \frac{F}{2} e^{ik_1 a} \cdot e^{-k_2 a} \qquad ...(viii)$$

Substituting these values of C and D in (v) and (vi) we get,

$$A = \frac{F}{4}e^{ik_{1}a} \left[\left(1 + \frac{k_{2}}{ik_{1}} \right) \left(1 + \frac{ik_{1}}{k_{2}} \right) e^{-k_{2}a} + \left(1 - \frac{k_{2}}{ik_{1}} \right) \left(1 - \frac{ik_{1}}{k_{2}} \right) e^{k_{2}a} \right]$$

$$= \frac{F}{4}e^{ik_{1}a} \left[\left(2 + \frac{k_{2}^{2} - k_{1}^{2}}{i k_{1}k_{2}} \right) e^{-k_{2}a} + \left(2 - \frac{k_{2}^{2} - k_{1}^{2}}{i k_{1}k_{2}} \right) e^{k_{2}a} \right]$$

$$= \frac{F}{4}e^{ik_{1}a} \left[2\left(e^{k_{2}a} + e^{-k_{2}a} \right) + \frac{k_{1}^{2} - k_{2}^{2}}{ik_{1}k_{2}} \left(e^{k_{2}a} - e^{-k_{2}a} \right) \right]$$
or
$$A = \frac{F}{4}e^{ik_{1}a} \left[4\cosh k_{2}a + \frac{2(k_{1}^{2} - k_{2}^{2})}{i k_{1}k_{2}} \sinh k_{2}a \right] \qquad \dots (51a)$$
and
$$B = \frac{F}{4}e^{ik_{1}a} \left[2\left(k_{1}^{2} + k_{2}^{2} \right) \sinh k_{2}a \right] \qquad \dots (51b)$$

SOME SIMPLE APPLICATIONS OF THE SCHROEDINGER'S EQUATION

Now we distinguish the following two cases:

(I) $E \subset K_0$; both the numbers k_1 and k_2 will be real in this case. The transmission coefficient is given by,

 $T = \frac{\text{Magnitude of transmitted current}}{\text{Magnitude of incident current}}$

$$= \frac{\hbar k_1}{m} |F|^2 / \frac{\hbar k_1}{m} |A|^2 = \frac{|F|^2}{|A|^2}$$

Using (51a) we can write,

$$T = \frac{16}{\left| \frac{4\cosh k_2 a + 2(k_1^2 - k_2^2)}{ik_1 k_2} \sinh k_2 a \right|^2}$$

$$= \frac{16 k_1^2 k_2^2}{16k_1^2 k_2^2 \cosh^2 k_2 a + 4(k_1^2 - k_2^2)^2 \sinh^2 k_2 a}$$

$$=\frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 \cosh^2 k_2 a + (k_1^2 - k_2^2)^2 \sinh^2 k_2 a} \qquad \dots (52)$$

Similary, the coefficient of reflection,

$$R = \frac{\text{Magnitude of the reflection current}}{\text{Magnitude of the incident current}} = \frac{|B|^2}{|A|^2}$$

$$= \frac{4(k_1^2 + k_2^2)^2 \sinh^2 k_2 a}{16k_1^2 k_2^2 \cosh^2 k_2 a + 4(k_1^2 - k_2^2)^2 \sinh^2 k_2 a}$$

$$= \frac{(k_1^2 + k_2^2)^2 \sinh^2 k_2 a}{4k_1^2 k_2^2 \cosh^2 k_2 a + (k_1^2 - k_2^2)^2 \sinh^2 k_2 a} \qquad ...(53)$$

Since k_1 and k_2 are real, therefore, T and R both are real. From the classical theory, a particle with energy less than V_0 will always be reflected, and there should not be any penetration of the barrier. But here we see that due to wave nature, the particle has finite probability of penetration through the barrier. This phenomenon is called the *tunnel effect*". It should be noted that the tunnel effect is purely a quantum mechanical concept.

Now let us consider a special case when the barrier is thick i. e., a very large, then $k_2a > 1$, and hence

sinh
$$k_2 a = \frac{e^{k_2 a} - e^{-k_2 a}}{2} \simeq \frac{e^{k_2 a}}{2}$$

and
$$\cosh k_2 a = \frac{e^{k_2 a} + e^{-k_2 a}}{2} \simeq \frac{e^{k_2 a}}{2}$$

Hence the approximate expression for T can be written as:

$$T \simeq \frac{16k_1^2 k_2^2 e^{-2k_2 a}}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2}$$

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Using the values of k_1 and k_2 from eqns. (49) we can write

$$T \simeq \frac{16E(V_0 - E)}{V_0^2} \exp \left[-2\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\right] a$$
 ...(54)

(II). $E \geqslant V_0$. In this case k_2 will be purely imaginary. We write, $k_1 = i \sqrt{\frac{2m(E - V_0)}{\hbar^2}} = ik'_2$ (say); k'_2 is real.

: $\sinh k_2 a = \sinh i \ k'_2 a = i \sin k'_2 a$ and $\cosh k_2 a = \cosh i k'_2 a = \cos k'_2 a$.

Therefore, the coefficient of transmission and the coefficient of reflection are given by,

$$T = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 \cos^2 k_2^2 a + (k_1^2 + k_2^2) \sin^2 k_2^2} \dots (55)$$

and

$$R = \frac{(k_1^2 - k'_2^2)^2 \sin^2 k'_2 a}{4k_1^2 k'_2^2 \cos^2 k'_2 a + (k_1^2 + k'_2^2)^2 \sin^2 k_2 a} \qquad \dots (56)$$

Since k_1 and k'_2 are real, both of T and R will also be real. Now the classical theory predicts that the particle will always be transmitted for energies greater than V_0 , while according to quantum mechanics the particle has a finite probability for reflection also.

Using the values of k_1 and k'_2 in (55) & (56) we can write,

$$T = \frac{4E (E - V_0)}{V_0^2 \sin^2 k'_2 a + 4E(E - V_0)}$$

$$R = \frac{V_0^2 \sin^2 k'_2 a}{V_0^2 \sin^2 k'_2 a + 4E(E - V_0)}$$

and

If the energy of the particle equals to height of the potential barrier, ie. if $E=V_0$, we have

$$T_0 = \left(1 + \frac{m\alpha^2 V_0}{2\hbar^2}\right)^{-1} \text{ and } R_0 = \left(1 + \frac{2\hbar^2}{m\alpha^2 V_0}\right)^{-1}$$

The barrier becomes completely transparant (R=0, T=1) if $\sin k'_2 a = 0$, i.e. if

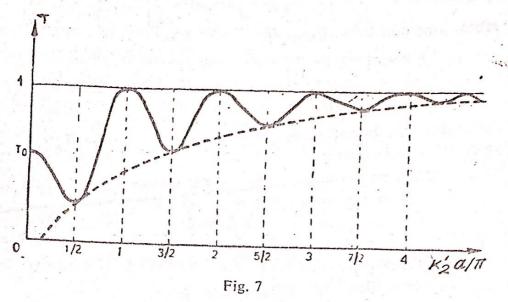
$$k'_2 a = n\pi$$
, $n = 1, 2, 3, ...$

or

$$a = \frac{n\pi}{k'_2} = n \frac{\lambda}{2}, n = 1, 2, 3, ...$$

Thus the passage of particles through rectangular barriers leads to resonance phenomena of a type unknown in classical physics (Fig. 7.)

It is analogous to the well known phenomenon of total transmission of light through a thin refraction layer, perfect



transmission occurs whenever the barrier width a is an integral number of half wavelengths.

PROBLEMS

Problem 1. Find the energies of the bound states of a particle in the symmetrical potential well given by

$$V(x) = \begin{cases} -V_0 & \text{for } |x| < a, \\ 0 & \text{for } |x| > a, \end{cases}$$

where V_0 is a positive quantity.

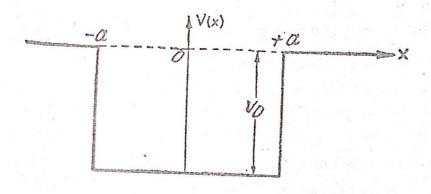


Fig. 8

Sol. For the existence of the bound state, the total energy E of the particle should be such that $-V_0 < E < 0$. The Schroedinger equation can then be written as

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2} |E| \psi = 0 \quad \text{for } x > a \text{ and } x < -a. \quad \dots \text{(ia)}.$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (V_0 - |E|) \psi = 0 \text{ for } |x| < a. \quad ...(ib)$$

Using the notations $\alpha = \sqrt{\left(\frac{2m \mid E \mid}{\hbar^2}\right)}$ and $\beta = \sqrt{\left(\frac{2m(V_0 - \mid E \mid)}{\hbar^2}\right)}$, the wavefunctions can be written as

$$\psi = Ae^{\alpha x} + Be^{-\alpha x}$$
, if $x > a$,
 $\psi = C \sin \beta x + D \cos \beta x$, if $|x| < a$,
 $\psi = Fe^{\alpha x} + Ge^{-\alpha x}$, if $x < -a$.

For ψ to describe bound states, we have to take A=G=0 (the vanishing condition at infinity).

From the continuity condition at $x=\pm a$, we obtain

$$2C \sin \beta a = (B - F)e^{-\alpha a}$$

$$2\beta C \cos \beta a = -\alpha (B - F) e^{-\alpha a}$$
, ...(iia)

$$2D \cos \beta a = (B+F) e^{-\alpha a}$$

$$2\beta D \sin \beta a = \alpha (B+F) e^{-\alpha a}$$
...(iib)

If $C \neq 0$, and thus $B \neq F$, we obtain from (iia)

$$\beta \cot \beta a = -\alpha$$
. ...(iii)

If $D\neq 0$, and thus $B\neq -F$, we obtain from (iib)

$$\beta \tan \beta a = \alpha$$
. ...(iv)

The relations (iii) and (iv) cannot be satisfied at the same We have therefore to distinguish two classes of solutions:

(I) C=0, B=F and $\beta \tan \beta \alpha = \alpha$.

(II) D=0, B=-F and β cot $\beta a=-\sigma$.

The corresponding energy values are given by the solutions If it trascondental equation (iii) and (iv), which can be solved graphically as follows.

Put $x = \beta a$ and $y = \alpha a$, the energy levels $E = -\frac{\hbar^2}{2ma^2}y^2$ are then obtained from the intersections of the curves

$$x \tan y = y$$

$$x^2 + y^2 = \frac{2ma^2}{\hbar^2} V_0$$

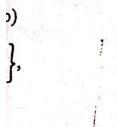
 $x \cot x = -y$

$$\begin{cases} x \cot x = -y \\ x^2 + y^2 = \frac{2ma^2}{\hbar^2} V_0 \end{cases}$$

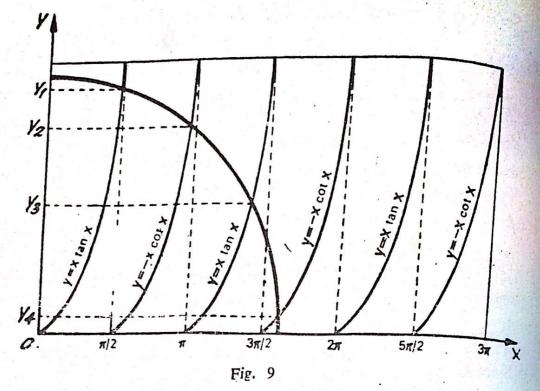
and

respectively in the regions x > 0 and y > 0 (see figure 9 on next page).

We can see from the figure that the number of bound states increases as the product a^2V_0 (the "well parameter") in-



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creases, and is finite if a^2V_0 is finite. It can also be seen that if $\frac{n\pi}{2} \leqslant R < \frac{(n+1)\pi}{2}$, where $R = \left(\frac{2m}{\hbar^2} a^2V_0\right)^{1/2}$ and n=0, 1, 2, ..., then the number of bound states is (n+1) (for n=0, the condition becomes $0 < R < \frac{1}{2}\pi$).

Problem 2. Soive the above problem when the potential well is not symmetric, i.e.,

$$V(x) = \begin{cases} -V_0 & \text{for } 0 < x < a \\ 0 & \text{for } x < 0 \text{ and } x > a. \end{cases}$$

Sol. The wavefunction in this case can be written as:

$$\psi = Be^{-\alpha x}, \quad \text{if } x > a,$$

$$\psi = C \sin \beta x + D \cos \beta x, \quad \text{if } 0 < x < a,$$

$$\psi = Fe^{\alpha x}, \quad \text{if } x > 0.$$

From the continuity condition at x=0 and x=a, we obtain

$$D = F, \qquad ...(a)$$

$$C \sin \beta a + D \cos \beta a = Be^{-\alpha a}, \qquad ...(b)$$

$$\beta C = \alpha F, \qquad ...(c)$$

$$\beta C \cos \beta a - \beta D \sin \beta a = -\alpha Be^{-\alpha a} \qquad ...(d)$$

From (a) and (c), D=F and $C=\frac{\alpha}{\beta}F$. Putting these values of D and C in (b) and (d) and then dividing one by the other, we get

after a little algebra

$$2 \cot \beta a = \frac{\beta}{\alpha} - \frac{\alpha}{\beta}. \qquad \qquad \dots (i)$$

Introducing the quantities

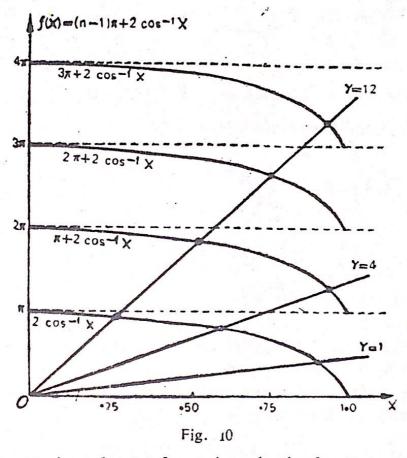
$$\gamma = \sqrt{\left(\frac{2mV_0a^2}{\hbar^2}\right)}, x = \frac{\beta a}{\gamma} = \sqrt{\left(1 - \frac{|E|}{V_0}\right)},$$

we can express (i) as

$$\gamma \dot{x} = (n-1) \pi + 2 \cos^{-1} x, n=1, 2,...$$
 ...(ii)

Figure below illustrates the transcendental equations (ii) graphically for the three cases $\gamma = 1$, 4, 12. The roots of it give the energy levels

$$E = -V_0 (1-x^2)$$
...(iii)



The number of states for a given depth of well is clearly the greatest integer contained in the quantity $\left(\frac{\gamma}{\pi}+1\right)$. This quantity increases as V_0 is made larger. The values of E corresponding to the stationary states decrease as the depth of well increases, and a new level appears at zero energy each time γ assumes the value $n\pi$.

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Problem 3. Solve the problem of article 5.4 by taking the well as a symmetric one,

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ V_0 & \text{for } |x| > a. \end{cases}$$

Sol. The wavefunction are given by

$$\psi = A \cos k_1 x + B \sin k_1 x \quad (-a < x < a),$$

$$\psi = Ce^{k_2x} \quad (x < -a),$$

$$\psi = De^{-k_2 x} (x > a),$$

where
$$k_1 = \sqrt{\left(\frac{2mE}{\hbar^2}\right)}$$
 and $k_2 = \sqrt{\left\{\frac{2m(V_0 - E)}{\hbar^2}\right\}}$

From continuity condition at $x=\pm a$, we obtain

$$A\cos k_1 a + B\sin k_1 a = De^{-k_2 a},$$

$$-k_1 A \sin k_1 a + k_1 B \cos k_1 a = -k_2 D e^{-k_2 a}$$

$$A\cos k_1 a - B\sin k_1 a = Ce^{-k_2 a}$$

 $k_1 A \sin k_1 a + k_1 B \cos k_1 a = k_2 C e^{-k_2 a}$

Solving these we obtain,

$$2A \cos k_1 a = (C+D) e^{-k_2 a},$$

$$2k_1 A \sin k_1 a = k_2 (C+D) e^{-k_2 a},$$
...(i)

$$2B \sin k_1 a = (D - C) e^{-k_2 a}$$

$$2k_1 B \cos k_1 a = -k_2 (D - C) e^{-k_2 a}$$
...(ii)

If $A \neq 0$ and $C \neq -D$, we obtain from (i) that

$$k_1 \tan k_1 a = k_2$$
. ...(iii)

If $B\neq 0$ and $C\neq D$ we obtain from (ii) that

$$k_1 \cot k_1 a = -k_2$$
. ...(iv)

The solutions (iii) and (iv) cannot be satisfied at the same time. We have therefore, to distinguish two classes of solutions;

(I) A=0, C=-D and $k_2 \cot k_1 a = -k_2$.

(II) B=0, C=D and $k_1 \tan k_1 a=k_2$.

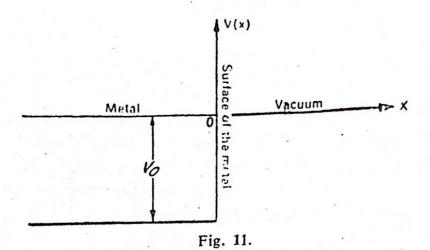
Solutions for these two cases can be found exactly in the same way as in Problem 1.

Problem 4. The conduction electrons in metals are held inside the metal by an average potential called the inner potential of the metal. Calculate, for the one-dimensional model given by $V(x) = -V_0$ if x < 0 and V(x) = 0 if x > 0, the probability of

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reflection and of transmission of a conduction electron approaching the surface of the metal with total energy E, (I) if E > 0 and (II) if $-V_0 < E < 0$.



Sol. The Schroedinger equation can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E + V_0) \psi = 0 \quad (x < 0),$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad (x > 0).$$

Defining
$$k_1 = \sqrt{\left\{\frac{2m(E+V_0)}{\hbar^2}\right\}}$$
 and $k_2 = \sqrt{\left(\frac{2mE}{\hbar^2}\right)}$, the wave-

functions can be written as

$$\psi = Ae^{ik_1x} + Be^{-ik_1x} (x < 0),$$

$$\psi = Ce^{ik_2x} + De^{-ik_2x} (x > 0).$$

For x < 0, the first term of ψ represents a wave which arrives at the surface from the left; *i.e.*, the incident wave and the second term represents the reflected wave. For x > 0, the first term of ψ represents the transmitted wave and the second term represents a represents the transmitted wave and the second term represents a wave arriving at the surface from the right. Since such a wave does not exist under the conditions of this problem we put D=0.

The continuity conditions at x=0 then yield the equations

$$A+B=C$$

$$k_1 (A-B)=k_2 C$$

whence we get it

$$B = \frac{k_1 - k_2}{k_1 + k_2} A, \quad C = \frac{2k_1}{k_1 + k_2} A \qquad ...(i)$$

Thus the reflection and the transmission co-efficients can be written as:

$$R = \frac{|S_R|}{|S_I|} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(\sqrt{E + V_0} - \sqrt{E})^2}{(\sqrt{E + V_0} + \sqrt{E})^2} \qquad \dots (ii)$$

$$T = \frac{\left| \frac{S_T}{S_I} \right|}{\left| \frac{S_T}{S_I} \right|} = \frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{4\sqrt{\{E(E + V_0)\}}}{(\sqrt{\{E + V_0\}} + \sqrt{\{E\}})^2} \qquad \dots \text{(iii)}$$

- (I) When E > 0, both of k_1 and k_2 are real and R is finite. Thus there is a finite probability for reflection even when E > 0 while from classical mechanics the particle should be completely transmitted.
- (II) If $-V_0 < E < 0$, the total energy of the electron is not sufficient for it to leave the metal, according to classical mechanics. In fact, in this case:

$$k_1 = \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}, k_2 = i\sqrt{\frac{2m|E|}{\hbar^2}},$$

and the solution bounded in the region x > 0 is

$$\psi = Ce^{-(x/2d)}$$
, where $d = \hbar (8m \mid E \mid)^{-1/2}$.

The continuity conditions at x=0 give

$$A+B=C$$

$$ik_1 (A-B) = -\frac{1}{2d} C$$

whence

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$$\frac{B}{A} = -\frac{1+2i \ k_1 d}{1-2i \ k_1 d}, \frac{C}{A} = -2 \ \frac{2i \ k_1 d}{1-2i \ k_1 d}.$$

From the wavefunction for x > 0 we see that $S_T = 0$, and hence T = 0 and $R = |B|^2 / |A|^2 = 1$. Thus, as in classical theory, an electron having a total energy smaller than the potential barrier height will be reflected with certainty. A new result however, is that the probability of finding the electron outside the metal (x > 0) is different from zero, since

$$|\psi(x)|^2 = 4 |A|^2 \left(1 + \frac{1}{4k_1^2 d^2}\right)^{-1} e^{-x/d} = 4 |A|^2 \frac{V_0 - |E|}{V_0} e^{-x/d}$$

N.B. Actually the potential energy does not jump from $-V_0$ to C at the metal-vacuum interface in such an abrupt manner. Its change is continuous over an interval of the order of the interatomic distances in the metal. However, the above type of simple picture of the actual potential can explain the qualitative features of the problem in a quite successful manner.

Problem 5. A beam of mono-energetic electrons strikes the surface of a metal at normal incidence. Calculate the reflection probability of these electrons if E=0.1 eV and $V_0=8$ eV.

Sol. Since the electrons with energy 1 e.V encounter a potential drop -8 e.V at the metal surface, they will all enter the metal, according to classical mechanics, and, because of the law of conservation of energy, they will acquire a final momentum $k_1 = \sqrt{\frac{\{2m \ (E+V_0)\}}{\hbar}}$ after doing so.

According to quantum mechanics, on the other hand, some of the electrons may be reflected by the metal surface. Using the notations of the last problem, $D \exp (-ik_2x)$ now represents the incident wave, $C \exp (ik_2x)$ the reflected wave and $B \exp (-ik_1x)$ the transmitted wave inside the metal. In this case A=0. The continuity conditions at the point x=0 give

$$C+D=B$$

$$k_2 (C-D)=-k_1 B,$$

whence

$$R = \frac{|S_R|}{|S_I|} = \frac{|C|^2}{|D|^2} = \left(\frac{k_2 - k_1}{k_2 + k_1}\right)^2$$

and

$$T = \left| \frac{S_T}{S_I} \right| = \frac{|B|^2}{|D|^2} = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

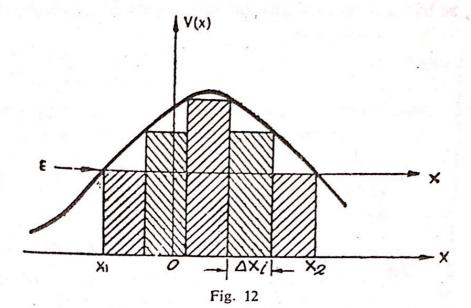
Thus, for E=0.1 e.V. and $V_0=8$ e.V., we have

$$R = \left\{ \frac{\sqrt{(E) - \sqrt{(E + V_0)}}}{\sqrt{(E) + \sqrt{(E + V_0)}}} \right\}^2 = \left[\frac{1 - \sqrt{(1 + V_0/E)}}{1 + \sqrt{(1 + V_0/E)}} \right]^2 = \left(\frac{8}{10} \right)^2 = 64$$

Problem 6. A particle of total energy E enters the barrier V=V(x) (shown in fig. 12) at the point $x=x_1$ and leaves it at the point $x=x_2$. Assuming the potential energy curve V(x) to be sufficiently smooth, calculate the approximate value of the transmission coefficient T.

Sol. Let us divide the interval $[x_1, x_2]$ into intervals of length $\triangle x_i$, large compared with the relative penetration depth $d_i = \sqrt{\left[\frac{\hbar^2}{8m \{V(x_i) - E\}}\right]}$ of a particle in the rectangular barrier so obtained. Then from article 5.6 we know that the transmission coefficient T_i for the *i*th rectangular barrier is given by

$$T_i \approx \exp\left[-2\sqrt{\left(\frac{2m\{V(x_i)-E\}}{\hbar^2}\right)\cdot \triangle x_i}\right]$$
 ...(i)



Hence the transmission co-efficient through the whole barrier will be given by the product

$$T = \prod_{i} T_{i} = \exp\left[-2\sum_{i} \sqrt{\left(\frac{2m\left\{V\left(x_{i}\right) - E\right\}}{\hbar^{2}}\right)} \cdot \triangle x_{i}\right] \qquad \dots (ii)$$

Increasing the subdivision of the interval x_1 , x_2 as far as is allowed by the condition $d_i << \triangle x_i$, the approximate formula,

$$T = \exp\left[-2\int_{x_1}^{x_2} \sqrt{\left(\frac{2m \{V(x) - E\}}{\hbar^2}\right)} dx\right] \qquad \dots \text{(iii)}$$

is obtained; this expression is known as "Gamow's penetrability factor".

Remarks: The above phenomenon of penetration of a barrier V = V(x) can be used to give some qualitative features of the theory of α -decay. The α -particles inside the nucleus are bound by tremendous and enormous attractive forces which are very similar to those involved in the attraction of neutrons and protons. However, these attractive forces have a very short range and these are negligible unless the α -particle is inside the nucleus. Outside the nucleus, α -particle experiences very strong coloumb repulsive forces. Therefore if an α -particle is brought from a long distance towards the nucleus, it will at first be repelled electrically and will posses potential energy $\frac{(2e)(Ze)}{r}$ where Ze is the charge on the nucleus, 2e is the charge on α -particle and r is the

distance of the α -particle from the centre of the nucleus. When this α -particle reaches the nucleus, the attractive forces dominate over the repulsive forces. The potential energy curve as a function of r will be of the form as shown below in figure 13.

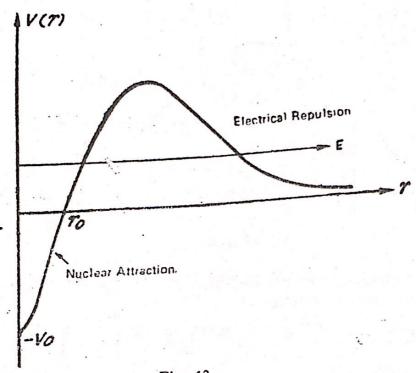


Fig. 13.

Now the α -particle can move freely inside the nucleus with velocity v_1 and kinetic energy

$$\frac{1}{2}mv_1^2 = E + V_0.$$

Since the α -particle is held inside the nucleus of radius r_0 by a potential barrier it will "collide" with this barrier $\frac{v_1}{2r_0}$ times per second. Each time it strikes the barrier, the probability of penetration of the barrier is equal to the transmission coefficient T. Thus the α -particle has a small but finite probability of penetrating the barrier even when its energy E is much less than that required to carry it over the barrier.

Problem 7. Approximating the nuclear potential by a square well type of potential, calculate the transmission probability for α -particles of energy N through the barrier. Express the result in terms of the final velocity of the α -particle, and estimate the mean life of an α -emitting nucleus.

SOME SIMPLE APPLICATIONS OF THE SCHROEDINGER'S EQUATION

Sol. From the last problem we have the probability of transmission

on
$$T = \exp \left[-2 \int_{r_0}^{r_1} \sqrt{\left(\frac{2m\left(V(r) - E\right)}{\hbar^2}\right) dr}\right] \qquad \dots (i)$$

$$E = \frac{(2e)\left(Ze\right)}{r_1} = \frac{2Ze^2}{r_1} \qquad \dots (ii)$$

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where

Changing the variable r to $r_1 \cos^2 x$ we get

Changing the Tangenty Theorem 1. Changing the Tangenty Theorem 2. The exp.
$$\left[\frac{-\sqrt{(8mE)} \int_{r_0}^{r_1} \sqrt{\left(\frac{r_1}{r} - 1\right) dr} \right]$$

$$= \exp \left[-\frac{\sqrt{(32mE)} \int_{0}^{r_1} r_1 \int_{0}^{\cos^{-1} r_0/r_1} \sin^2 x \, dx \right]$$

$$= \exp \left[-\frac{\sqrt{(16mZe^2 r_1)}}{\hbar} \left\{ \cos^{-1} \left(\frac{r_0}{r_1}\right)^{1/2} - \sqrt{\left(\frac{r_0}{r_1}\right) \cdot \sqrt{\left(1 - \frac{r_0}{r_1}\right)} \right\} \right]$$

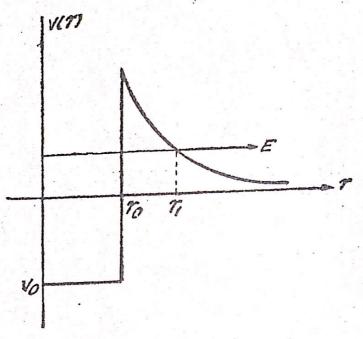


Fig. 14.

Now the α -particles having energies of a few MeV can leave potential wells of depth of tens of MeV, inside which they find themselves in radioactive nuclei, we can take $E < < V(r_0)$, i.e., $r_0 < < r_1$. We can, thus neglect terms of higher order than the first in $\left(\frac{r_0}{r_1}\right)^{1/2}$ and obtain

ADVANCED QUANTUM THEORY AND FIELDS
$$T = \exp \left[-\frac{\sqrt{(16mZe^2)}}{\hbar} \cdot \left(\frac{\pi}{2} \sqrt{(r_1)} - \sqrt{(r_0)} \right) \right]$$

$$= \exp \left[\frac{\sqrt{(16mZe^2 r_0)}}{\hbar} - \frac{1}{v} \frac{4\pi Ze^2}{\hbar} \right] \qquad \dots \text{(iii)}$$
which we have put $\pi = 2Ze^2$

in which we have put $E = \frac{2Zc^2}{r_1} = \frac{mv^2}{2}$, v being the velocity of the α -particle at a large distance r from the nucleus for which

Using eqn. (iii) for T, the mean life τ of an α -particle emitting nucleus can be estimated as follows: We have remarked before this problem that the α -particle collides the barrier, $\frac{v_1}{2r_0}$, times per second and (iii) gives the probability for penetration per collision. Hence the probability per unit time of the α-particle lea-

$$\frac{1}{\tau} = \frac{v_1}{2r_0} T$$

Using (iii) we obtain finally.

$$\ln \tau = \left\{ \frac{1}{2} \ln \frac{2r_0^2 m}{V_0} - \sqrt{\left(\frac{(16mZe^2 r_0)}{\hbar^2}\right) + \frac{4\pi Ze^2}{\hbar} \cdot \frac{1}{v}} \right\} \qquad \dots (iv)$$
This relation size

This relation gives an estimate of the mean life τ of an lpha-emitting nucleus in terms of the lpha-particle velocity v at large distances and the nuclear radius r_0 .

Problem 8. If a beam of electrons impinges on an energy barrier of height 0.03 eV and of infinite width, find the fraction of electrons reflected and transmitted at the barrier if the energy of the impinging

Sol. This is the problem of a square potential step barrier. In case-I. $E > V_0$. E=0.04 e.V. and $V_0=0.03 \text{ e.V.}$

The reflection coefficient R is given by

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{[\sqrt{(E)} - \sqrt{(E - V_0)}]^2}{[\sqrt{(E)} + \sqrt{(E - V_0)}]^2} = \frac{[\sqrt{(0.04)} - \sqrt{(0.01)}]^2}{[\sqrt{(0.04)} + \sqrt{(0.01)}]^2} \approx 0.1.$$
The transmission of the first series of the series

The transmission coefficient is given by,

$$T=1-R\approx 0.9$$
.

In case-II. $E < V_0$.

The transmission coefficient is zero and hence the reflection coefficient is one.

In the last case $E=V_0$. Therefore, $k_2=0$.

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = 1$$

and **

T=0.

Problem 9 Calculate the probability of transmission of a proton through the barrier indicated below:

$$V_0=2$$
 eV, $E=1$ eV and barrier width=1 Å.

Sol. The probability of transmission is given by $T = \frac{16 E(V_0 - E)}{V_0^2} e^{\left[-2\sqrt{2m(V_0 - E)}\right] a/\hbar}$

Here $V_0=2 \text{ eV}=2\times1.6\times10^{-12} \text{ ergs.}$ $E=1 \text{ eV}=1.6\times10^{-12} \text{ ergs.}$ $m=1.6\times10^{-24} \text{ gm., } a=10^{-8} \text{ cm.}$ $h=1.05\times10^{-27} \text{ erg-Sec.}$ $T=4e^{-\frac{1}{13}}$

Problem 10. Calculate the probability of transmission for 1 MeV proton through a 4 MeV high and 10^{-12} cm. thick rectangular potential barrier.

[Do as the previous problem. Ans. 0.0015].

 $V_0 = 4 M e V$ $A = 10^{-12} cm$ $T = 16 E (V_0 - E) [-2 \sqrt{2} m (r_0 - E)]^2 a/k$

T= 1/2/h, 1/2 (10/2+ 10:2)

Bound state problems are those in which the particle is restrained by the external forces (potential energy) to a particular region of space. For example, the one dimensional motion of a point mass attached to a fixed centre, *i.e.*, linear harmonic oscillator is one of the fundamental problems of bound states. Similarly, the hydrogen atom in which one electron is moving around the positively charged nucleus is of great importance in quantum mechanics. The aim of this chapter is to solve the Schroedinger equation for some important bound state problems.

6.1. ONE DIMENSIONAL LINEAR HARMONIC OSCILLATOR:

The one dimensional linear harmonic oscillator is a point mass attached to a fixed centre by a force which is proportional to its displacement. The study of simple harmonic oscillator is ery important and useful because a number of more complicated stems can be analysed with its help. For example the vibrations of an elastic medium or electromagnetic field in a cavity can be described by superposition of an infinite number of simple harmonic oscillator.

The potential energy V(x) in case of linear harmonic oscillator is expressed by

$$V(x) = \frac{1}{2}kx^2, \qquad \dots(1)$$

$$(: F = -kx)$$

Therefore the Schroedinger wave equation can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2}kx^2\right) \psi = 0. \tag{2}$$

Introducing a dimensional independent variable ρ*

$$\rho = \alpha x$$
 with $\alpha = \left(\frac{m\omega_c}{\hbar}\right)^{1/2}$,

^{*}Note that α has the dimension of the inverse of the length and hence ρ is dimensional independent variable,

where $\omega_c = (k/m)^{1/2}$ is the angular frequency of the corresponding classical harmonic oscillator, we have

$$\frac{d^2\psi}{d\rho^2} + (\lambda - \rho^2) \psi = 0, \qquad \dots (3)$$

$$\lambda = \frac{2E}{\hbar^2} \left(\frac{m}{k}\right)^{1/2} = \frac{2E}{\hbar w_0}.$$

where

Now we have to find the solutions of equation (3) which do not diverge at infinity. For $\lambda=1$, the solution of equation (3) is of the form $\psi(\rho)=e^{-\rho^2/2}$. For other values of λ , it is reasonable to expect that the asymptotic behaviour of $\psi(\rho)$ would be of the same nature because as $\rho \to \pm \infty$, the constant λ becomes insignificant compared to ρ^2 . Thus the solution of equation (3) may be taken of the form

$$\psi(\rho) = H(\rho) e^{-\rho^2/2} , \qquad \dots (4)$$

where H(P) is a polynomial of finite order in P.

Substitution of equation (4) in equation (3) gives

$$H''-2\rho H'+(\lambda-1) H=0,$$
 ...(5)

where primes denote differentiation with respect to ρ .

Energy Levels. We try a power series expansion in ρ for $H(\rho)$

$$H(\rho) = \rho^{s} (a_0 + a_1 \rho + a_2 \ell^2 + ...) a_0 \neq 0, s \geqslant 0$$

or

$$H(\rho) = \sum_{\nu=0}^{\infty} a_{\nu} e^{s+\nu}, \qquad ... (6)$$

Substituting the values of H, H' and H'' from equation (6) in equation (5), we get

$$\sum_{\nu} a_{\nu} (s+\nu) (s+\nu-1) \rho^{s+\nu-2} - 2 \sum_{\nu} a_{\nu} (s+\nu) \rho^{s+\nu} + (\lambda-1) \sum_{\nu} a_{\nu} \rho^{s+\nu} = 0.$$
...(7)

As the right-hand side of equation (7) is zero, the coefficient of each power of ρ must be identically equal to zero. Equating the coefficients of ρ^{s-2} , ρ^{s-1} , ρ^s , ρ^{s+1} and $\rho^{s+\nu}$ to zero, we get

$$s(s-1) a_0 = 0,$$
 ...(8)

$$(s+1) sa_1=0,$$
 ...(9)

$$(s+2) (s+1) a_2 - (2s+1-\lambda) a_0 = 0,$$
 ...(10)

$$(s+3) (s+2) a_3 - (2s+3-\lambda) a_1 = 0,$$
 ...(11)

$$(s+\nu+2)(s+\nu+1)a_{\nu+2}-(2s+2\nu+1-\lambda)a_{\nu}=0.$$
 ...(12)

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From equation (8), we have s=0 or s=1 beacuse $a_0\neq 0$. From (11) gives us the recursion formula,

$$\frac{a_{\nu+2}}{a_{\nu}} = \frac{2s + 2\nu + 1 - \lambda}{(s + \nu + 2)(s + \nu + 1)} \qquad \dots (13)$$

Now we choose λ in such a way that the power series for $H(\rho)$ Now we have the series to break off after the causes the series to break off after the series the series to break off after the series the series the serie cuts on at some the series to break off after the nth term is seen which causes (13) to be from equation (13) to be ...(14)

$$\lambda = 2s + 2v + 1. \qquad \dots (14)$$

The index s can still be either 0 or 1. When s=0, $\lambda=2\nu+1$ and when s=1, $\lambda=2\nu+3$, where ν is an even integer. We may and whom express both cases in terms of a quantum number n, ...(15)

$$\lambda = (2n+1). \qquad \dots (15)$$

i.e.,

$$\lambda = \frac{2E}{\hbar\omega_c}$$

Again

Hence the general expression for energy is given by ...(16) $E_n = (n + \frac{1}{2}) \hbar \omega_c$.

Zero point energy. The energy levels given by equation (16) are discrete levels as they have equal spacing. The finite non-zero value of ground state energy level (corresponding to n=0 $\frac{1}{2}$. $\hbar\omega_c$ is known as zero point energy. Thus the zero point energy is given by ...(17)

$$E_0 = \frac{1}{2}\hbar \omega_c. \qquad ...(17)$$

Zero point energy is a characteristic of quantum mechanics and is related to uncertainty principle as was seen in Problem 16 of Chapter 1.

Harmonic Oscillator Wavefunctions. Since $\lambda = (2n+1)$, equation (5) is now of the form

$$H''_{n}(\rho) - 2\rho H'_{n}(\rho) + 2nH_{n} = 0. \tag{18}$$

The polynomials $H_n(\rho)$ are called as Hermite polynomials.

The general solution is given by

$$\psi_n(\rho) = N_n H_n(\rho) e^{-\rho^2/2}, \qquad ...(19)$$

where N_n is a constant.

To obtain the value of this constant, we consider a generating function $e^{-s^2+2s\rho}$ which is given by

$$e^{-s^{2}+2s\rho} = \sum_{n=0}^{\infty} \frac{H_{n}(\rho)}{n!} s^{n}.$$
 ...(20)

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Similarly,
$$e^{-t^2+2t\rho} = \sum_{m=0}^{\infty} \frac{H_m(\rho)}{m!} t^m$$
. ...(21)

Now consider the product of these two generating functions, which is given by

$$\int_{-\infty}^{+\infty} e^{-s^2+2s\rho} \cdot e^{-t^2+2t\rho} d\rho$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n}{n!} \cdot \frac{t^m}{m!} \int_{-\infty}^{+\infty} H_n(\rho) H_m(\rho) d\rho.$$

Multiplying by $e^{-\rho^2}$ on both the sides we have $\int_{-\infty}^{+\infty} e^{-s^2+2s\rho} \cdot e^{-t^2+2t\rho} \cdot e^{-\rho^2} d\rho$

$$=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{s^{n}}{n!}\cdot\frac{t^{m}}{m!}\int_{-\infty}^{+\infty}H_{n}\left(\rho\right)H_{m}\left(\rho\right)e^{-\rho^{2}}d\rho.$$
...(22)

The integral of left hand side is given by

The integral of left hand side is given by
$$\int_{-\infty}^{+\infty} e^{-s^2 + 2s\rho} \cdot e^{-t^2 + 2t\rho} \cdot e^{-\rho^2} d\rho$$

$$= \int_{-\infty}^{+\infty} \exp\left\{-s^2 - t^2 + 2s\rho + 2t\rho - \rho^2\right\} d\rho$$

$$= e^{2st} \int_{-\infty}^{+\infty} e^{-(\rho - s - t)^2} d(\rho - s - t)$$

$$= e^{2st} \cdot \sqrt{(\pi)}$$

$$= \sqrt{(\pi)} \left[1 + \frac{2st}{1!} + \frac{(2st)^2}{2!} + \dots + \frac{(2st)^n}{n!}\right]$$

$$= \sqrt{(\pi)} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!}.$$

Equating equal powers of s and t on both the sides, we get

$$\int_{-\infty}^{+\infty} H_n^2(\rho) e^{-\rho^2} d\rho = \sqrt{(\pi)} \, 2^n \, n \, ! \text{ when } n = m$$

$$\int_{-\infty}^{+\infty} H_n(\rho) \, H_m(\rho) \, e^{-\rho^2} \, d\rho = 0 \text{ if } m \neq n.$$

and

Now applying the normalization condition, we have

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = \frac{|N_n|^2}{\alpha} \int_{-\infty}^{+\infty} H_n^2(\rho) e^{-\rho^2} d\rho = 1$$

$$\frac{|N_n|^2}{\alpha} \cdot \sqrt{(\pi) \cdot 2^n} \; n \; !=1.$$

$$N_n = \left[\frac{\alpha}{\sqrt{(\pi) \cdot 2^n n!}}\right]^{1/2}.$$

Substituting this value of N_n in equation (19), the normalized wave functions of harmonic oscillators are given by

$$\psi_n(\rho) = \left\{ \frac{\alpha}{\pi^{1/2} \cdot 2^n \ n!} \right\}^{1/2} H_n(\rho) \ e^{-\rho^2/2}. \tag{23}$$

Physical Interpretation of Harmonic Oscillator Wavefunctions:

The wavefunction $\psi_0(\rho)$ for the ground state of harmonic oscillator and the corresponding probability distribution function $[\psi_0(\rho)]^2$ as a function of ρ are shown in figure 1 (a) and (b).

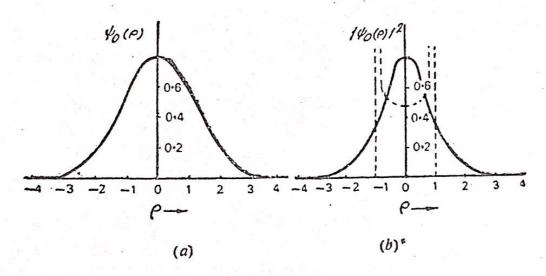
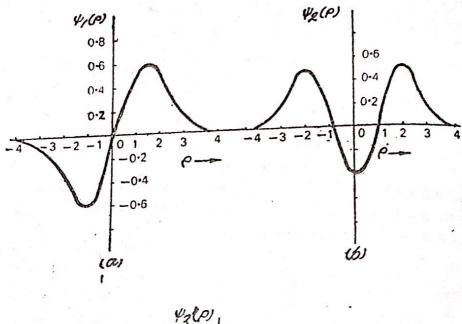


Fig. 1. Wavefunction ψ_0 (ρ) as a function of ρ for ground state for harmonic oscillator.

 $|\psi_0(\rho)|^2$ as a function of ρ . Classical distribution curve is shown by dotted curve.

It is obvious from fig. 1 (b) that the quantum mechanical result for this case does not agree at all with the classical result. According to the classical theory, for a given energy there is a limit beyond which the oscillator cannot go and the classical probability density approaches infinity at this limit. Quantum mechanically, on the other hand, there is a small probability outside this region. This feature is a characteristic of quantum mechanics and is closely connected with the Heisenberg's uncertainty relation.

Figure 2 shows the form of ψ_n (ρ) for larger value of n.



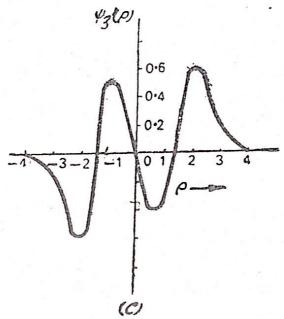
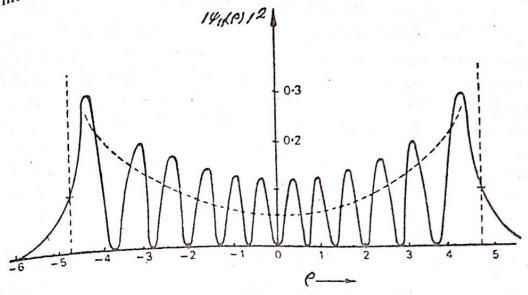


Fig. 2.

Figure 3 shows the variation of $\psi^2(\rho)$ as a function of ρ for the state n=11 with the classical probability curve for the same energy. The classical curve is shown by dotted line. It is observed that apart from the fluctuations in the curved obtained quantum mechanically, there is a general agreement between the two functions. This kind of correspondence does not exist for every small n but improves rapidly with increasing n.

The number of zeros (i.e., points where the probability is zero except for the end points) in the nth excited state of the oscillators

are equal to n and all of them are contained within the classical interval.



Probability density for the harmonic oscillator in state ψ_{11} (ρ). The dotted curve represents the classical probability dissribution.

Probability Inside and Outside the Classical Region in (Ground State).

The wavefunctions of harmonic oscillator are given by

$$\psi_{n}(\rho) = \left\{ \frac{\alpha}{\sqrt{(\pi)} \frac{1}{2} 2^{n} n!} \right\}^{1/2} H_{n}(\rho) e^{-\rho^{2}/2}.$$

In the ground state
$$\psi_0(\rho) = \left(\frac{\alpha}{\sqrt{(\pi)}}\right)^{1/2} e^{-\rho^2/2}$$
. ...(24)

The classical probability is given by

$$\int_{-a}^{+a} |\psi_0|^2 dx = 2 \int_0^a \frac{\alpha}{\sqrt{\pi}} e^{-\rho^2} dx$$

$$= 2 \int_0^a \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2} dx. \qquad ...(25)$$

In quantum mechanics, the probability is given by

$$P=2\int_{0}^{+1/\alpha}\frac{\alpha}{\sqrt{\pi}}.e^{-\alpha^{2}x^{2}} ax.$$

Putting $\alpha x = \rho$, we get

$$P = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-\rho^2} d\rho$$

$$= \frac{2}{\sqrt{\pi}} \int_0^1 \left[1 - \frac{\rho^2}{1!} + \frac{\rho^4}{2!} - \frac{\rho^6}{3!} + \frac{\rho^8}{4!} \right] d\rho$$

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$$= \frac{2}{\sqrt{\pi}} \left[\rho - \frac{\rho^3}{3.1!} + \frac{\rho^5}{5.2!} - \frac{\rho^7}{7.3!} + \frac{\rho^9}{9.4!} \right]_0^1$$

$$= \frac{2}{\sqrt{\pi}} \left[1 - \frac{1}{3.1!} + \frac{1}{5.2!} + \frac{1}{7.3!} + \frac{1}{9.4!} \right]_0^1$$

$$= 0.83$$

$$= 83\%$$

Thus the probability of finding the oscillator inside the classical limit is 83% while outside the classical limit is 17%.

6.2: THREE DIMENSIONAL HARMONIC OSCILLATOR:

A three dimensional harmonic oscillator consists of a particle bound to the origin by the force having components $-k_x x$, $-k_y y$ and $-k_z z$ along X, Y and Z axes respectively. Here k_z , k_y and k_z and the force constants in the three directions and x, y and z are the components of the displacement along the three axes.

The potential energy of the system is

$$V = \frac{1}{2} k_x x^2 + \frac{1}{2} k_y y^2 + \frac{1}{2} k_z z^2. \qquad ...(1)$$

The Schroedinger wave equation for this system is

The Schröddinger wave equation
$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{2m}{\hbar^2} \left[E - \frac{1}{2} k_x x^2 - \frac{1}{2} k_y y^2 - \frac{1}{2} k_z z^2 \right] \psi = 0. \tag{2}$$

Let
$$\lambda = \frac{2mE}{\hbar^2}$$
, $\alpha_x^2 = \frac{mk_x}{\hbar^2}$, $\alpha_y^2 = \frac{mk_y}{\hbar^2}$ and $\alpha_z^2 = \frac{mk_z}{\hbar^2}$

On substitution, eqn. (2) becomes

On substitution, eqn. (2) becomes
$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + [\lambda - (\alpha_x^2 x^2 + \alpha_y^2 y^2 + \alpha_z^2 z^2)] \psi = 0 \qquad (3)$$

Eqn. (3) can be resolved into three separate equations by the method of separation of variables. Let us substitute

$$\psi = X(x) Y(y) Z(z), \qquad ... (4)$$

where X(x), Y(y) and Z(z) are functions of x, y and z only.

Substituting eqn. (4) in eqn. (3), we get,

$$\left(\frac{1}{X}\frac{d^{2}X}{dx^{2}}-\alpha_{x}^{2}x^{2}\right)+\left(\frac{1}{Y}\frac{d^{2}Y}{dy^{2}}-\alpha_{y}^{2}y^{2}\right)+\left(\frac{1}{Z}\frac{d^{2}Z}{dz^{2}}-\alpha_{z}^{2}z^{2}\right)+\lambda=0$$
...(5)

From eqn. (5), we have

$$\left(\frac{1}{X}\frac{d^2X}{dx^2} - \alpha_x^2 x^2\right) + \lambda_x = 0$$

$$\left(\frac{1}{Y}\frac{d^2Y}{dy^2} - \alpha_y^2 y^2\right) + \lambda_y = 0 \qquad \dots (6)$$

$$\left(\frac{1}{Z}\frac{d^2Z}{dz^2}-\alpha_z^2z^2\right)+\lambda_z=0$$

Where $\lambda = \lambda_x + \lambda_y + \lambda_z$.

Eqn. (6) can be written as

$$\frac{d^2X}{dx^2} + \left(\lambda_x - \alpha_x^2 x^2\right) X = 0 \qquad \dots (7)$$

$$\frac{d^2Y}{dy^2} + \left(\lambda_y - \alpha_y^2 y^2\right) Y = 0 \qquad \dots (8)$$

$$\frac{d^2Z}{dz^2} + \left(\lambda_z - \alpha_z^2 z^2\right) Z = 0 \qquad \dots (9)$$

The components of energy values are given by

$$E_x = \left(n_x + \frac{1}{2}\right) \hbar \omega_x$$
, $E_y = \left(n_y + \frac{1}{2}\right) \hbar \omega_y$ and $E_z = \left(n_z + \frac{1}{2}\right) \hbar \omega_z$.

Here n_x , n_y and n_z are non negative integers.

The energy eigen values of three dimensional harmonic oscillator are given by,

$$E = E_x + E_y + E_z$$

$$= [(n_x + \frac{1}{2}) \omega_x + (n_y + \frac{1}{2}) \omega_y + (n_z + \frac{1}{2}) \omega_z] \hbar \qquad ...(10)$$

For a special case of isotropic oscillator, in which $\omega_x = \omega_y = \omega_z$ and $\alpha_x = \alpha_y = \alpha_z$, eqn. (10) reduces to

 $E = [(n_x + n_y + n_z + \frac{3}{2}) \ \omega] \ \hbar = (n + \frac{3}{2}) \ \hbar \omega,$...(11) where $n = n_x + n_y + n_z$ may be called as the total quantum number. The wavefunctions are given by,

$$X(x) = \left[\frac{\alpha_x}{\sqrt{\pi \cdot 2^{n_x} n_x}}\right]^{1/2} e^{-\alpha_x^2 x^2/2} H_{n_x} (\alpha_x x)$$

$$Y(y) = \left[\frac{\alpha_y}{\sqrt{\pi \cdot 2^{n_y} n_y}}\right]^{1/2} e^{-\alpha_y^2 y^2/2} H_{n_y} (\alpha_y y) \qquad \dots (12)$$

$$Z(z) = \left[\frac{\alpha_z}{\sqrt{\pi \cdot 2^{n_z} n_z}}\right]^{1/2} e^{-\alpha_z^2 z^2/2} H_{n_z} (\alpha_z z)$$

The complete normalised wave function is given by

$$\psi = \left[\frac{\alpha_x \alpha_y \alpha_z}{n^{8.2} 2^{(n_x + n_y + n_z)} n_x ! n_y ! n_z !}\right]^{1/2} e^{-\frac{1}{2}(\alpha_x^2 x^2 + o_y^2 y^2 + \alpha_z^2 z^2)} \times H_{n_x}(\alpha_x x) H_{n_y}(\alpha_y y) H_{n_z}(\alpha_z z) \dots (13)$$

As the energy of this system depends only on the total quantum numbers, all the energy levels except the lowest one are degenerate. The degeneracy is (n+1) (n+2)/2.

6.3. SPHERICALLY SYMMETRIC SYSTEMS AND POTEN. TIALS:

Spherical symmetric systems are those in which the potential energy of the particle is only a function of radius vector and is independent of θ and ϕ . We now take the case of hydrogen atom which consists of an atomic nucleus of charge +e and electron of charge -e. We are interested in the motion of two particles (nucleus and electron) that are attracted by a force which depends only on the distance r between them. If the nucleus is supposed to be at rest, then the Schroedinger eqn is the same as that for a single particle in which the mass m is replaced by the reduced mass μ . The potential energy is given by,

$$V(r) = -e^2/r.$$

Such potentials are known as spherically symmetric potentials.

6.4. SEPARATION OF VARIABLES:

The Schroedinger wave equation is given by

$$\nabla^2 \psi + \frac{2m}{\hbar^2} \left[E - V \right] \psi = 0 \qquad \dots (1)$$

In case of spherical polar coordinates, we have

$$x = r \sin \theta \cos \phi,$$

$$y = r \sin \theta \sin \phi,$$

$$z = r \cos \theta,$$
and
$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\frac{r^2 \partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \theta^2}$$

Thus the Schroedinger wave equation with spherically symmetric potential may be written in spherically coordinates as

The potential may be written in
$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(\frac{r^2 \partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{\hbar^2} \left[E - V(r) \right] \psi = 0.$$
 ...(3)

In order to separate eqn. (3), let us express $\psi(r, \theta, \phi)$ as the product of three functions viz. R(r), $\Theta(\theta) \Phi(\phi)$, each of which is a function of one indicated variable,

$$i e., \qquad \psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi). \qquad ...(4)$$

Substitution eqn. (4) in eqn. (3) and simplifying, we get

$$\frac{1}{R} \frac{d}{dr} \left(\stackrel{\mathcal{V}}{r} \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[E - V(r) \right]$$

$$= -\frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) - \frac{1}{\Phi \sin^2 \theta} \frac{d^2 \Phi}{d\phi^2} \qquad ...(5)$$

The left hand side is a function of r while the right hand side is a function of θ and ϕ . This is only possible when they are separately equal to a constant quantity say λ .

$$\therefore \frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[E - V(r) \right] = \lambda,$$

or

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[\frac{2m}{\hbar^2}\left\{E - V(r)\right\} - \frac{\lambda}{r^2}\right]R = 0 \qquad ...(A)$$

The right hand side of eq. (5) can be written as

$$\frac{1}{\Theta} \sin \theta \, \frac{d}{d\theta} \left(\sin \theta \, \frac{d\Theta}{d\theta} \right) + \lambda \sin^2 \theta = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \qquad \dots (6)$$

The left hand side of eq. (6) is only a function of θ , while right hand side is a fauction of ϕ . Let they are separately equal to a constant m^2 , hence

$$-\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m^2$$

$$\frac{d^2 \Phi}{d\phi^2} + m^2 \Phi = 0 \qquad \dots (B)$$

or

and

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \left(\lambda - \frac{m^2}{\sin^2 \theta} \right) \Theta = 0 \qquad \dots (C)$$

In this way the wave equation is separated in three variables.

6.5. THE HYDROGEN ATOM:

Hydrogen atom is a system of two interacting point charges, the positively charged nucleus and the negatively charged electron. The schroedinger wave equation for hydrogen atom in spherical polar coordinates can be written as

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{\partial r} \right) + \frac{1}{r^2 \sin \psi} \frac{d}{d\theta} \left(\sin \psi \frac{d\psi}{d\theta} \right) + \frac{1}{r^2 \sin^2 \psi} \frac{d^2\psi}{d\phi^2} + \frac{2\mu}{\hbar^2} \left[E - V(r) \right] \psi = 0 \qquad \dots (1)$$

Where μ is reduced mass and $V(r) = -e^2/r$. Separating this equation in three variables, we have

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[\frac{2\mu}{\hbar^2}\left\{E + \frac{e^2}{r}\right\} - \frac{\lambda}{r^2}\right]R = 0 \qquad \dots (2)$$

$$\frac{d^2\Phi}{d\psi^2} + m^2\Phi = 0 \qquad \dots (3)$$

and

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin \frac{d\Theta}{d\theta} \right) + \left(\lambda - \frac{m^2}{\sin^2\theta} \right) \Theta = 0 \qquad ...(4)$$

The solution of Φ equation. The solution of eq. (3) can be written as

$$\Phi_{\mathfrak{m}} = \frac{1}{\sqrt{(2\pi)}} e^{i\mathfrak{m}\phi} \qquad \dots (6)$$

Where the constant $m=0, \pm 1, \pm 2, ...$ and is called the magnetic quantum number.

The solution of Θ equation. Let us define a new variable x such that $x=\cos\theta$. Substituting this in eq. (4), we have

$$\frac{d}{dx}\left\{(1-x^2)\frac{d\Theta}{dx}\right\} + \left\{\lambda - \frac{m^2}{(1-x^2)}\right\}\Theta = 0 \qquad \dots (7)$$

For $\lambda = l$ (l+1), where l=0, 1, 2, 3 ... called as azimutal quantum number, the solution of eq. (7) is given by

$$\Theta_{lm} = \left[\frac{(2l+1). \ l \ |m|!}{2. \ l+|m|!} \right]^{1/2} P_{l}^{lml} (\cos \theta) \qquad .. (8)$$

where $P_{l^{|m|}}$ is called the associated Legendre function

The solution of radial equation. The radial part is given by

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2\mu}{\hbar^2} \left\{ E + \frac{e^2}{r} \right\} - \frac{l(l+1)}{r^2} \right] R = 0$$

Now we introduce a dimensionless independent variable

$$\rho = \alpha r$$
 or $r = \rho/\alpha$

The radial equation takes the form

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left[\frac{2\mu E}{\hbar^2 \alpha^2} + \frac{2\mu e^2}{\hbar^2 \alpha \rho} - \frac{l(l+1)}{\rho^2} \right] R = 0 \qquad \dots (9)$$

According to classical mechanics, the negative energies $(E\langle 0)$ correspond to elliptical orbits representing bound states in an atomic system; while the positive energies (E > 0) correspond to hyperbolic orbits representing unbound states. In this case let us consider that the electron is bound in hydrogen atom *i.e.*, E < 0. Thus for bound state (E < 0) we have E = -|E|. The eq. (9) can be written as

$$\frac{1}{\rho^{2}} \frac{d}{d\rho} \left(\frac{dR}{d\rho} \right) + \left[- \left[\frac{2\mu}{\hbar^{2}x^{2}} + \frac{2\mu e^{2}}{\hbar^{2}\alpha\rho} - \frac{l(l+1)}{\rho^{2}} \right] R = 0 \quad ...(10)$$

We choose $a^2 = \frac{8u \mid E \mid}{\hbar^2}$

and set

$$\lambda = \frac{2\mu \ e^2}{\hbar^2 \alpha} = \frac{e^2}{\hbar} \left(\frac{2}{2 |E|} \right)^{1/2}$$

Thus eq, (10) becomes

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] R = 0 \qquad \dots (11)$$

If $p \to \infty$, eq. (11) is of the form

$$\frac{d^2R}{d\rho^2} = \frac{1}{4}R.$$

The solution of this equation is $R = e^{+\rho/2}$ and $R = e^{-\rho/2}$.

As ρ may vary from 0 to ∞, the former of these solutions will increase as ρ increases. This leads to an unacceptable wavefunction. On the other hand second solution decreases to zero as ρ and hence r increases to infinity. Consequently the second solution is satisfactory. This suggests that we look for an exact solution of eq. (11) of the from

$$R(\rho) = F(\rho) e^{-\rho/2},$$
 ...(12)

where $F(\rho)$ is a polynomial of finite order in ρ .

Substitution of eq. (12) in eq. (11) gives

$$\frac{d^{2}F}{d\rho^{2}} + \left(\frac{2}{\rho} - 1\right) \frac{dF}{d\rho} + \left[\frac{(\lambda - 1)}{\rho} - \frac{l(l + 1)}{\rho^{2}}\right] F = 0 \dots (13)$$

Energy levels. We now try a series solution of eq. (13) of the form

$$F(\rho) = \sum_{r=0}^{\infty} a_r \, \rho^{s+r} \qquad \dots (14)$$

Substituting the values of F(P), dF/dP, and d^2F/dP^2 from eq. (14) in eq. (13) we get.

$$\sum_{r=0}^{\infty} [(s+r) (s+r-1) + 2 (s+r) - l (l+1)] a_r \rho^{s+r} - \sum_{r=0}^{\infty} [(s+r) - (\lambda - 1)] a_r \rho^{s+r+1} = 0$$

$$-\sum_{r=0}^{\infty} [(s+r) - (\lambda - 1)] a_r e^{s+r+1} = 0 \qquad ...(15)$$

Comparing the coefficients of Ps on both sides of eq. (15) we get

$$\begin{array}{ccc}
[s (s+1)-l (l+1)] & a_0=0 \\
\text{or} & s(s+1)-l (l+1)=0 \\
\text{which yield } s=l & \text{or } s=-(l+1)
\end{array}$$
: $a_0 \neq 0$

The value of s = -(l+1) does not satisfy the condition of well behaved function and hence the only accepted value of s is l.

Comparing the coefficients of ρ^{g+r+1} on both sides of eq. (15), the following recurrence formula is obtained

$$\frac{a_{r+1}}{a_r} = \frac{s+r+1-\lambda}{(s+r+1)(s+r+2)-l(l+1)} \dots (16)$$

The condition that the series breaks off after finite number of terms is

$$\lambda = n = \eta' + l + 1 \tag{17}$$

where n' is the value of r for which the series terminates.

Since n' and l can be positive integer or zero, n can have values 1, 2, 3 The number n is called the total quantum number. The energy eigen values are given by

$$\lambda = \frac{e^2}{\hbar} \left(\frac{\mu}{2 |E|} \right)^{1/2} \quad \text{or } n = \frac{e^2}{\hbar} \left(\frac{\mu}{2 |E|} \right)^{1/2}$$

$$E_n = -|E_n| = -\frac{\mu e^4}{2n^2 \hbar^2}. \quad \dots (18)$$

This value agrees with the value obtained by old quantum theory and by experiment.

Radial wave functions. We now consider the solution of eq. (13) in the form

$$F(\rho) = \sum_{r=0}^{\infty} a_r \ \rho^{s+r} = \rho^s L(\rho) \qquad \dots (19)$$

Substitution of eq. (19) in eq. (13) gives

$$e^{2}L'' + e[2(s+1)-e]L' + [e(\lambda-s-1)]$$

$$+s(s+1)-l(l+1)]L=0,$$

Putting s=l and $\lambda=n$, we have

$$PL'' - [2(l+1) - P]L' + (n-l-1)L = 0$$
 ...(20)

We know that the associated Laguerre equation is

$$e L_q^{p''} + (p+1-e) L_q^{p'} + (q-p) L_q^p = 0$$
 ...(21)

The solution of eq. (21) is L_q^p . Hence the solution of eq. (20)

can be expressed in terms of associated Laguerre polynomials. Comparing eq. (20) with eq. (21), we have

$$p+1=2(l+1)$$
 or $p=2l+1$ and $q-p=n-l-1$ or $q=n+l$

Thus the solution of eq. (20) can be expressed as $L_{n+1}^{2l+1}(\rho)$

The radial wave function is now of the form

$$R(\rho) = F(\rho) e^{-\rho/2} = \rho^s L_{n+l}^{2l+1} (\rho) e^{-\rho/2}$$

or
$$R(\rho) = \rho^{l} e^{-\rho/2} L_{n+l}^{2l+1}(\rho)$$
 ...(22)

The normalized radial wave function is given by

$$R(\rho) = C \rho^{1} e^{-\rho/2} L_{n+l}^{2l+1} (\rho) \qquad ...(23)$$

where C is normalization constant. The value of C can be obtained as follows:

$$C^{2}\int_{0}^{\infty}e^{-\rho} \rho^{2l} \left[L_{n+l}^{2l+1}(\rho)\right]^{2} \rho^{2} d\rho = 1$$

Solving we get
$$C = \left[\left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n \{(n+l)!\}^3} \right]^{1/2}$$

Where $a_0 = \frac{\hbar^2}{\mu e^2}$ and $\rho = \frac{2r}{na_0}$

$$R_{n_l}(r) = \left[\left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n \{(n+l)!\}^3} \right]^{1/2}$$

$$e^{-r/na_0} \left(\frac{2r}{na_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right) \qquad \dots (24)$$

The first three radial wave functions are

$$R_{10}(r) = \left(\frac{1}{a_0}\right)^{3/2} 2 e^{-r/a_0}$$

$$R_{20}(r) = \left(\frac{1}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$R_{21}(r) = \left(\frac{1}{2a_0}\right)^{3/2} \frac{r}{a_0 \sqrt{3}} e^{-r/2a_0} \qquad \dots(25)$$

Complete wavefunctions. The complete wavefunctions of hydrogen atom are given by

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r) \Theta_{ml}(\theta) \Phi_{m}(\phi)$$

$$= \left[\left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n \{(n+l)!\}^3} \right]^{1/2} e^{-r/na_0} \left(\frac{2r}{na_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right)^l \\
\times \left[\frac{2l+1}{2} \frac{l-|m|!}{l+|m|!} \right] P_l^m(\cos\theta) \times \frac{1}{\sqrt{(2\pi)}} e^{im\phi} \dots (26)$$

The wavefunctions for various values of n, l and m are given below

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n	l I	m	State	Eigen function
1	0	0	1 <i>s</i>	$\psi_{100} = \frac{1}{\sqrt{(\pi)}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$
2	0	0	2s	$\psi_{200} = \frac{1}{4\sqrt{(2\pi)}} \left(\frac{1}{a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2u_0}$
2	1	0	2 <i>p</i>	$\psi_{210} = \frac{1}{4\sqrt{(2\pi)}} \left(\frac{1}{a_0}\right)^{5/2} e^{-r/2a_0} r \cos \theta$
2	1	1	2 <i>p</i>	$\psi_{211} = \frac{1}{4\sqrt{(2\pi)}} \left(\frac{1}{a_0}\right)^{5/2} e^{-r/2a_0} \sin \theta e^{i\phi}$

66. DEGENERACY:

Except for n=1, each energy level is degenerate, being

represented by more than one independent solution of the wave equation. The allowed values of quantum numbers are:

Total quantum number $n=1, 2, 3, \ldots$

Azimuthal quantum number $l=0, 1, 2, 3 \dots (n-1)$

Magnetic quantum number m=-l, -l+1, -l+2, ...-1, 0, +1, ... l-1, l.

Thus there are (2l+1) independent wavefunctions for a given value of n and l and n^2 independent wavefunctions with a given value of n as can be seen below

$$\sum_{l=0}^{n-1} (2l+1) = 2 \sum_{l=0}^{n-1} l + \sum_{l=0}^{n-1} (1)$$

$$= 2 \frac{(n-1) n}{2} + n = n^2 - n + n = n^2.$$

The degeneracy with respect to m is the characteristic of central force field *i.e.*, the force field depending only on the radial distance r, while the degeneracy with respect to l is characteristic of Coulomb field. In presence of some external field such as a magnetic field, (2l+1) fold m degeneracy disappears and the level is split up into n^2 different energy levels.

6.7. THE GROUND STATE OF HYDROGEN ATOM:

In the ground state n=1, l=0 and m=0. The wavefunction is given by

$$\psi_{100} = \frac{1}{\sqrt{\{(\pi a_0^3)\}}} e^{-r/a_0} \qquad ...(1)$$

The probability distribution function of the electron relative to nucleus is given by

$$\psi^*_{100} \psi_{100} = \frac{1}{\pi a_0^3} \cdot e^{-2r/a_0} \qquad ...(2)$$

As eq. (2) is independent of θ and ϕ , hence the normal hydrogen atom is spherically symmetric.

The probability that the electron will lie in a small volume $dV=r^2\sin\theta\ dr\ d\theta\ d\phi$ is given by

$$\psi^*_{100} \psi_{100} r^2 dr \sin \theta d\theta d\phi = \frac{1}{\pi a_0^3} e^{-2r/a_0^2} r^2 dr \sin \theta d\theta d\phi.$$
...(3)

The probability that the electron will lie between the distances r and r+dr from the nucleus irrespective of its angular distribution is given by

$$P(r) dr = \frac{1}{\pi a_0^3} e^{-2r/a_0} r^2 dr \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi$$
or
$$P(r) dr = \frac{4}{a_0^3} e^{-2r/a_0} r^2 dr \qquad ...(4)$$

Now the radial distribution function is given by

$$P(r) = \frac{4}{a_0^3} e^{-2r/a_0} r^2 \qquad ...(5)$$

For the most probable distance r, P(r) should be maximum i.e.,

$$\frac{d}{dr} P(r) = 0$$

$$\therefore \frac{d}{dr} \left[\frac{4}{a_0^3} e^{-2r/a_0} r^2 \right] = 0$$

This gives $r=a_0$ =radius of the first Bohr's orbit.

Thus the most probable distance of the electron from the nucleus in the normal state of hydrogen ctom is equal to Bohr's radius.

6.8. DISCUSSION OF HYDROGEN WAVE FUNCTIONS:

A plot of radial wave functions $R_{ni}(r)$ for n=1, 2 and 3 with l=0 and l=1 are shown in fig. (4). It can be observed from the figure that a wavefunction crosses the ρ axis (n-l-1) times in the region between $\rho=0$ and $\rho=\infty$. The corresponding planes are know as nodal planes. It can also be shown that the angular dependence of wave function further gives rise to l nodal planes. Thus the total nodal planes are $\lceil (n-l-1)+l \rceil = n-1$. These nodal planes, therefore, provides a new interpretation to n. Accordingly n gives the number of nodal planes but by one unit greater. probability distribution function $P = 4\pi r^2 [R_{nl}(r)]^2$ against ρ is shown in fig. (5). Here P represents the probability of finding the electron between two spheres of radii r and r+dr. It is obvious from the fig. (5) that 1S electron has the greatest probability at a0, i.e., the radius of first Bohr's orbit. Similarly the 2S electron has the greatest probability of being found at a distance about $5a_0$ than at any other distance.

The dependence of distribution on ϕ is given by $e^{im\phi}$ and is a constant. The probability distribution of all ψ_{nlm} is symmetric with respect to z-axis. The angular part of the wavefunction is given by the function $Y_{lm}(\theta, \phi)$. $|Y_{lm}(\theta, \phi)|^2$ for different values of $m[m=\pm l]$ has been plotted for various l values in fig. (6). It

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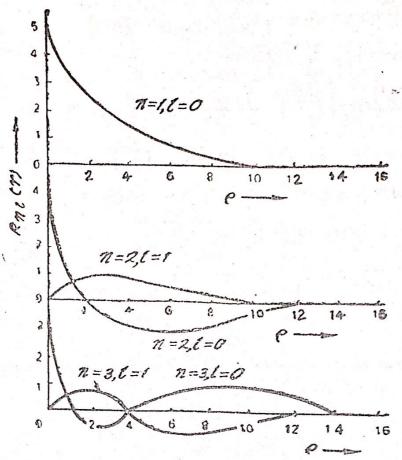


Fig. 4. Radial functions for hydrogen atom $R_{nl}(r)$ for n=1, 2, 3, and l=0 and 1.

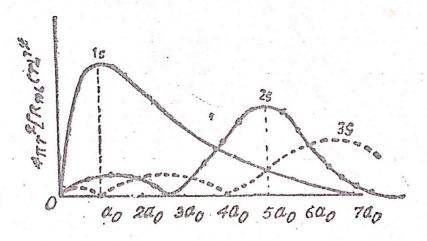


Fig. 5. Probability distribution function

can be observed from the figure that the probability distribution function becomes more and more concentrated about XY plane with the increase of l values. The behaviour of distribution function for other values of m is shown in fig. (7). It can be observed from fig. (7) that the function tend to be concentrated in directions corresponding to the plane of the oriented Bohr orbit. It also

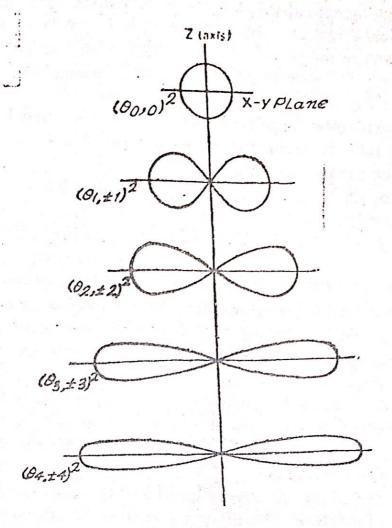


Fig. 6. $[Y_{lm}(\theta, \phi)]^2$ for various l values.

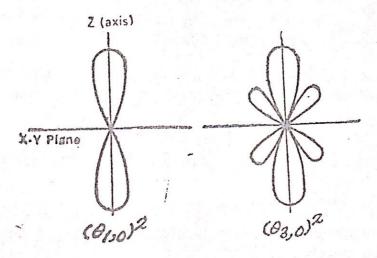


Fig. [7 (a)]

obvious that when [l-|m| is large, the curve representing θ_{lm} consists of a large number of lobes because the θ dependence of Θ has a wave like structure.

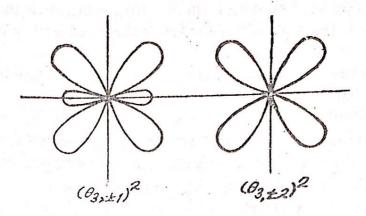


Fig. [7 (b)] Distyibution function for different I values.

6.9. QUANTUM NUMBERS:

The physical quantities in quantum mechanics, in general, are quantised. These quantities are prescribed by numbers and not by integers. The numbers are called as quantum numbers. Here we shall describe some quantum numbers.

1. The principal or total quantum number n. classically, the principal quantum number n represents the principal orbit to which the electron belongs. In terms of the principal quantum number n, the energy of the electron and its distance from the nucleus for hydrogen atom are given by

$$E_n = -\frac{13.6}{n^2} eV \text{ and } r_n = 0.529 n^2 \text{ Å}.$$

In quantum mechanics, the concept of definite orbit is discarded, even then n gives mean distance of an electron from the nucleus. The electron with n=1 is more nearer to the nucleus than electron with n=2. The total quantum number n can have only non-zero positive integral values, i.e., $n=1, 2, 3, \infty$. The principal quantum number is attached to a new meaning when we consider the probability distribution of the particle. In turns, it specifies the number of nodal surfaces (surface in which the particle has zero probability existence) greater in magnitude by one unit.

2. Orbital quantum number l. classically, this quantum number defines the shape of the orbital occupied by the electron and the orbital angular momentum of the electron. The orbitals corresponding to l=0, 1, 2, 3 etc. are designated as s, p, d, f etc. respectively. when n=1, l=0 there is only one possible orbital i.e., s orbital. For n=2, there are two possible orbitals i.e., s orbital and p orbital. Quantum mechanically, orbital quantum number l assumes the values $0, 1, 2, \ldots, (n-1)$ and specifies the

angular momentum the unit of \hbar or more correctly the angular momentum is written as $p_l = \sqrt{l(l+1)\hbar}$. The quantum number l governs the degree with which the electron is attached to the nucleus the larger is the value of l, weaker is the bond with which it is maintained with the nucleus

3. Spin quantum number s. This quantum number has been introduced to account for the spin of electrons about their own axis. The magnitude is always half. Since the electron can spin clockwise or anticlockwise, there are two values given to s, $+\frac{1}{2}$ and $-\frac{1}{2}$ depending upon whether the electron spins in one direction or the other. Two electron with same sign of spin quantum number are said to have parallel spins while with those have opposite spins of spin quantum numbers are said to have oppsite spins or paired up spins. Physically the letter s denotes the spin angular momentum in unit of h. In wave mechanics, its value is given by

$$p_s = \sqrt{s(s+1)} \hbar$$
.

4. Total angular quantum number j. This quantum number represents the resultant angular momentum of the electron due to both orbital and spin motions. It's numerical value is vector sum of l and s. It is usually expressed as $j = l \pm \frac{1}{2}$, plus sign is used when s is a parallel to l and minus when s is antiparallel to l. The angular momentum of a particle is written as

$$p_j = \sqrt{\{j(j+1)\}} \hbar.$$

5. Magnetic orbital quantum number m_l . When an atom is placed in a strong magnetic field, the electrons with same values of principal quantum number n and orbital quantum number l, may still differ in their behaviour. To account for, one more quantum number m_l , known as magnetic orbital quantum number has been introduced. According to the rule of space quantisation, the orientations of l with H are slimited and are determined by the fact that projection of l in the field direction assumes integral values. This projection of l in the field direction is known as magnetic orbital quantum number. Thus m_l assumes the values given by

$$m_l = l$$
, $(l-1)$, $(l-2)$... 0 , -1 , -2 , ... $(l-2)$, $(l-1)$, $-l$.

The maximum positive value of m_l is l and minimum is zero. There are in all (2l+1) values for m_l including zero.

6. Magnetic spin quantum number m_s . Just as vector I representing orbital angular momentum processes in the presence of

magnetic field, so does vector representing the spin angular m_0 mentum. The numerical value of m_s is the projection of spin vector s on field direction. By analogy with the orbital vector m_s can have any of the (2s+1) values from -s to +s excluding zero. However s is always equal to $\frac{1}{2}$ and never zero. This means that m_s can have only two values $+\frac{1}{2}$ and $-\frac{1}{2}$.

7. Magnetic total angular momentum quantum number m_j . Its numerical value is the projection of the total angular momentum vector j on the field direction. Since j can have half integral values, m_j can alo assume half integral values. The possible values of m_j are

$$-j$$
, $-(j-1)$, ... -1 , 0 , $+1$, ... $(j-1)$, j . i.e., $(2j+1)$ values in all.

6.10. THE RIGID ROTATOR:

A system of two spherical masses rigidly located at a finite fixed distance from one another and capable to rotate freely about its centre of mass is called a **rigid rotator with free axis**. A good idealization of it is a diatomic molecule with atoms of masses m_1 and m_2 located a distance r_0 apart, because the molecule can freely rotate about its centre of gravity. The theory of the rigid rotator will, therefore lead to the interpretation of the spectra of diatomic molecules.

In order to find out the energy levels and the corresponding eigenfunctions for the rigid rotator, we first write Schroedinger equation for it. The kinetic energy of the rotator is given by,

K.E.,
$$=\frac{p^2}{2\mu}$$
; where p is the momentum of the rotator and $\mu = \frac{m_1}{m_1 + m_2}$ is the reduced mass.

The moment of inertia of the rotator about an axis passing through the centre of mass and perpendicular to the line joining the two mases is given by,

$$I = \mu r_0^2$$

Using it, the kinetic energy of the rotator can be written as:

K. E.
$$=\frac{r_0^2}{2I}p^2$$
 ...(1)

Since the rotator can rotate freely, its potential energy is zero and hence the Hamiltonian, which is equal to the total energy, can be written as:

$$H=K. E.+P. E.=\frac{r_0^2}{2I}p^2+0$$
 ...(2)

replacing p^2 by its quantum mechanical operator, we get $H = \frac{-\ln^2 r_0^2}{2I} \nabla^2 \qquad ...(3)$

Hence, the Schroedinger equation $H\psi = E\psi$, can be written

as:
$$\frac{-\hbar^2 r_0^2}{2I} \nabla^2 \psi = E \psi \text{ or } r_0^2 \nabla^2 \psi + \frac{2IE}{\hbar^2} \psi = 0 \qquad \dots (4)$$

Since the rotator is rigid, there cann't be any radial variation of ψ , hence the eqn. (4) can be written in polar coordinates as:

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2IE}{\hbar^2} \psi = 0 \qquad ...(5)$$

In order to solve the Schroedinger equation (5) for rigid rotator, we apply the method of separation of variables, *i.e.* we write

$$\phi = \Theta(\theta)\Phi(\phi) \qquad \dots (6)$$

Substituting this in equantion (3) and dividing by $\Theta(\theta)\Phi(\phi)$ we get

$$\frac{1}{\Theta \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi \sin^2 \theta} \cdot \frac{\partial^2 \overline{\Phi}}{\partial \phi^2} + \frac{2IE}{\hbar^2} = 0 \qquad \dots (7)$$

Multiplying this equation by $\sin^2 \theta$, we get

$$\frac{\sin\theta}{\Theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial\Theta}{\partial\theta} \right) + \frac{1}{\Phi} \frac{\partial^2\Phi}{\partial\phi^2} + \frac{2IE}{\hbar^2} \sin^2\theta = 0$$

or
$$\frac{\sin \theta}{\Theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{2IE}{\hbar^2} \sin^2 \theta = -\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} \qquad \dots (8)$$

The left hand side of the above equation is a function of θ alone, while the r. h. s. is a function of ϕ alone, therefore, both sides must be equal to some constant, m^{\sharp} ((say). We thus obtain two differential equations:

$$\frac{d^{2}\Phi}{d\varphi^{2}} = -m^{2}\Phi \qquad \dots (9-a)$$

and
$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \left(\frac{2IE}{\hbar^2} - \frac{m^2}{\sin^2 \theta} \right) \Theta = 0$$
 ... (9-6)

The solution of equation 9-a is:

$$\mathfrak{D}(\varphi) = C_1 e^{\pm im\varphi} \qquad \dots (10)$$

where C_1 is an arbitrary constant.

In order that Φ may be single valued, we must have $\Phi(\varphi) = \Phi(\varphi + 2\pi)$. Therefore.

$$C_1 e^{\pm im\varphi} = C_1 e^{\pm im(\varphi + 2\pi)}$$
 or $e^{\pm im(2\pi)} = 1$
 $\vdots m = 0, \pm 1, \pm 2, \pm 3, ...,$ (11)

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We find the constant C such that Φ is normalized, i.e.,

$$\int_{0}^{2\pi} \Phi *\Phi d\varphi = 1$$

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$$C_1^2 \int_0^{2\pi} d\varphi = 1$$
 or $C_1^2 2 \pi = 1 \Rightarrow C_1 = \frac{1}{\sqrt{2\pi}}$

Thus the normalized functions are,

$$\bar{\Phi} = \frac{1}{\sqrt{2\pi}} e^{\pm im\varphi}, \text{ where } m=0, \pm 1, \pm 2, \dots \text{etc.}$$
 ...(12)

In order to solue equation (9-b), we put

$$\cos \theta = x$$

and

After substitutions equation (9-b) is transformed into the equation

$$(1-x^2) \frac{d^2\Theta}{dx^2} - 2x \frac{d\Theta}{dx} + \left(\frac{2IE}{\hbar^2} - \frac{m^2}{1-x^2}\right)\Theta = 0 \qquad ...(13)$$

Since m can take only integral values, equation (13) is exactly the Associated Legendre equation. The corresponding eigenvalues, the energy levels, are therefore given by

$$\frac{2IE}{\hbar^2} = l (l+1) \quad \text{or} \quad \left[= \frac{\hbar^2}{2I} l (l+1) \right] \qquad \dots (14)$$

where l= integer $\geqslant |m|$, and is called the principal or rotational quantum number.

The solution of equation (13) is given by

$$\Theta = C_2 P_1^m (x) \qquad \dots (15)$$

where,
$$P_i^m(x) = \frac{(1-x^2)^{m/2}}{2^i l!} \frac{d^{i+m}(x^2-1)^i}{dx^{i+m}}$$
, is the associated

Legendre polynomial and C_2 is a constant which may be chosen to normalize Θ . Therefor,

$$\int \Theta^* \Theta \ d\theta = 1$$
i.e., $C_2^2 \int_{-1}^{+1} P_l^m (x) P_l^m(x) dx = 1$

or
$$C_2^2$$
. $\frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} = 1$
from orthonormality properties of $P_i^m(x)$

$$\Rightarrow C_2 = \sqrt{\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m)!}}$$

Hence the normalized function Θ is given by

$$\Theta = \sqrt{\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m) l}} \cdot P_{l}^{m} (\cos \theta) \qquad \dots (16)$$

The complete wave functions or eigen-functions for the rigid rotator are given by

$$\psi = \Theta(\theta)\Phi(\varphi) = \sqrt{\frac{2l+1}{2} \frac{(l-m)!}{(l+m)!}} \cdot P_i^m \cos \theta \cdot \frac{1}{\sqrt{2n}} e^{\pm im\varphi}$$

or
$$\psi_{lm}(\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi} \cdot \frac{(l-m)!}{(l+m)!}} P_l^m (\cos \theta) e^{\pm im\varphi}$$
 ...(17)

Degeneracy. The energy eigenvalues of the rigid rotator, given by (14), depend only on l and are have degenerate with respect to m. For each value of l, m can take (2l+1) values from -l to +l. This means that there are (2l+1) possible wave-functions for each l, while there is only one energy value E_l for each l. Thus the system is (2l+1)—fold degenerate.

Rigid Rotator in a Fixed Plane. If we consider the rigid rotator in a fixed plane, say X-Y plane, then $\theta=90^{\circ}$. Hence, the Schroedinger equation (5), can be written as:

$$\frac{\partial^2 \psi}{\partial \varphi^2} + \frac{2IE}{\hbar^2} \psi = 0 \qquad \dots (18)$$

Writing $\frac{2IE}{\hbar^2} = m^2$, where m is some constant, we get, from (18) as:

$$\frac{\partial^2 \psi}{\partial \varphi^2} + m^2 \psi = 0 \qquad \dots (19)$$

The solution of equation (19) is given as:

 $\psi = Ce^{\pm im\varphi}$; where C is an arbitrary constant.

From the condition that ψ is single valued we get, m=0, ± 1 , ± 2 , ± 3 ,...., and from the normalization condition of ψ we get $C = \frac{1}{\sqrt{2\pi}}$. Thus, the normalized eigen functions are given by,

$$\psi = \frac{1}{\sqrt{2\pi}} e^{\pm im\varphi}, m=0, \pm 1, \pm 2, \dots$$
 ...(20)

The corrosponding eigenvalues are given from $\frac{2IE}{\hbar^2} = m^2$, as

$$E_m = \frac{\hbar^2 m^2}{2I}$$
, $m = 0, \pm 1, \pm 2, \dots$...(21)

This equation represents the rotational energy eigen values of the rigid rotator.

PROBLEMS

Problem 1. Calcuate the zero point energy of a system consisting of a mass of 1 gm. connected to a fixed point by a spring which is stretched 1 cm. by a force of 10,000 dynes, the particle being constrained to move only along X-axis

Sol. The zero point energy is given by $E = \frac{1}{2} \hbar \omega_0$,

where
$$\omega_0 = \sqrt{\left(\frac{K}{m}\right)}$$
.

According to the problem $K=10^4$ dynes and m=1 gm.

$$\omega_0 = \sqrt{\left(\frac{10^4}{1}\right)} = 10^2 \text{ sec}^{-1}.$$

Now $E_0 = \frac{1}{5} \times 1.05 \times 10^{-27} \times 10^2$ [: $h = 1.105 \times 10^{-27}$ erg. sec.] = 5.2×19^{-26} ergs.

Problem 2. Find the expectation value of the energy when the state of the harmonic oscillator is described by the following wave function.

$$\psi(x, t) = \frac{1}{\sqrt{(2)}} [\psi_0(x, t) + \psi_1(x, t)]$$

where $\psi_0(x, t)$ and ψ_l , (x, t) are the wavefunctions for the ground state and the first excited state respectively.

Sol. We know that the expectation value of energy E is given by

$$\langle E \rangle = \int \psi^* (x, t) E \psi (x, t) dx.$$
 ...(1)

Here

$$\psi(x, t) = \frac{1}{\sqrt{(2)}} \left[\psi_0(x, t) + \psi_1(x, t) \right]$$

i.e.,
$$\psi^*(x, t) = \frac{1}{\sqrt{(2)}} [\psi_0^*(x, t) + \dot{\psi}_1^*(x, t)]$$

The wavefunction in the ground state is given by

$$\psi_0(x,t) = \left(\frac{\alpha}{\sqrt{(\pi)}}\right)^{1/2} e^{-\alpha^2 x^2/2} \qquad ...(2)$$

The wavefunction in the first excited state is

$$\psi_1(x, t) = \left(\frac{\alpha}{2\sqrt{(\pi)}}\right)^{1/2} e^{-\alpha^2 x^2/2} 2\alpha x \qquad ...(3)$$

Now
$$\psi_0^*(x, t) = \left(\frac{\alpha}{\sqrt{(\pi)}}\right)^{1/2} e^{-\alpha^2 x^2/2} = \psi_0(x, t)$$
 ...(4)

and
$$\psi_1^*(x, t) = \left(\frac{\alpha}{2\sqrt{(\pi)}}\right)^{1/2} e^{-\alpha^2 x^2/2} . 2\alpha x = \psi_1(x, t)$$
 ...(5)

Therefore the value of

$$\psi^{*}(x, t) \psi(x, t) = \frac{1}{\sqrt{(2)}} [\psi_{0}^{*}(x, t) + \psi_{1}(x, t)]$$

$$\times \frac{1}{\sqrt{(2)}} [\psi_{0}(x, t) + \psi_{1}(x, t)]$$

$$= \frac{1}{2} [\psi_{0}(x, t) + \psi_{1}(x, t)]^{2}$$

$$= \frac{1}{2} [\psi_{0}(x, t) + \psi_{1}^{2}(x, t) + 2\psi_{0}(x, t) \psi_{1}(x, t)]$$

:. Expectation value of energy

$$\langle E \rangle = \frac{1}{2} \left[\int_{-\infty}^{+\infty} \psi_0^2(x, t) E_0 dx + \int_{-\infty}^{+\infty} \psi_1^2(x, t) E_1 dx + 2 \int_{-\infty}^{+\infty} \psi_0(x, t) \psi_1(x, t) E dx \right],$$

$$= \frac{1}{2} \left[\int_{-\infty}^{+\infty} \psi_0(x, t) \left(\frac{1}{2} \hbar \omega \right) dx + \int_{-\infty}^{+\infty} \psi_1^2(x, t) \left(\frac{3}{2} \hbar \omega \right) dx + 0 \right],$$

$$E_0 = \frac{1}{2} \hbar \omega, E_1 = \frac{3}{2} \hbar \omega \text{ and } \int_{-\infty}^{+\infty} \psi_0(x, t) \psi_0(x, t) E dx = 0$$

$$= \frac{1}{4} \hbar \omega \int_{-\infty}^{+\infty} \frac{\alpha}{\sqrt{(\pi)}} e^{-\alpha^2 x^2} dx$$

$$+ \frac{3}{4} \hbar \omega \int_{-\infty}^{+\infty} \frac{\alpha}{2\sqrt{(\pi)}} e^{-\alpha^2 x^2} 4\alpha^2 x^2 dx$$

$$= \frac{1}{4} \hbar \omega \frac{\alpha}{\sqrt{(\pi)}} \frac{\sqrt{(\pi)}}{\alpha} + \frac{3}{4} \hbar \omega \frac{\alpha}{2\sqrt{(\pi)}} 4\alpha^2 \frac{1}{2} \frac{\sqrt{(\pi)}}{\alpha^3}$$

$$= \frac{1}{4} \hbar \omega + \frac{3}{4} \hbar \omega = \hbar \omega.$$

Problem 3. Use the function $\psi = Nr^2 e^{-r/a_0}$ to construct a wave-function which is orthogonal to the ground state of hydrogen atom. N is a constant, which can be chosen as the normalization constant.

Sol. To find out N, we have

$$\int \psi^* \psi \ d^3r = 1,$$
i.e.
$$N^2 \int r^4 e^{-2r/a_0} r^2 \ dr \sin \theta \ d\theta \ d\psi = 1$$

$$4\pi N^2 \int_0^\infty r^6 e^{-2r/a_0} dr = 1$$
.

To evaluate the above integral, we use the standard integral,

$$\int_0^\infty r^n e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}}.$$

$$\therefore 4\pi N^2 \frac{6!}{(2/a_0)^7} = 1 \Rightarrow N^2 = \frac{2}{45\pi a_0^7} \text{ or } N = \sqrt{\left(\frac{2}{45\pi a_0^7}\right)}.$$

.. Normalized \(\psi \) can be written as

$$\psi = \frac{\sqrt{(2) \ r^2}}{\sqrt{(45\pi a_0^7)}} \ e^{-r/a_0}...(i)$$

The normalized ground state wavefunction for hydrogen atom is

$$\psi_{100} = \frac{1}{\sqrt{(\pi a_0^3)}} e^{-r/a_0}...(ii)$$

To find a wavefunction which is orthogonal to (ii), we use the Schmidt's method. Let

$$v_{1} = \psi_{100} = \frac{1}{\sqrt{(\pi a_{0}^{3})}} e^{-r/a_{0}}; u_{2} = \frac{\sqrt{(2)} r^{2}}{\sqrt{(45\pi a_{0}^{7})}} e^{-r/a_{0}}$$
and
$$v_{2} = u_{2} + a_{21}v_{1},$$
where
$$a_{21} = -(v_{1}, u_{2}) \quad \{ \because v_{1} \text{ is normalized, } \because (v_{1}, v_{1}) = 1 \}$$

$$= -\sqrt{\left(\frac{2}{45}\right)} \cdot \frac{1}{\pi a_{0}^{5}} \int_{0}^{\infty} r^{2} e^{-2r/a_{0}} d^{3}r$$

$$= -\sqrt{\left(\frac{2}{45}\right)} \cdot \frac{4\pi}{\pi a_{0}^{5}} \int_{0}^{\infty} r^{4} e^{-2r/a_{0}} dr$$

$$= -\sqrt{\left(\frac{32}{45}\right)} \cdot \frac{1}{a_{0}^{5}} \cdot \frac{4!}{(2/a_{0})^{5}} = -\sqrt{\left(\frac{2}{5}\right)}.$$

$$\therefore v_{2} = \sqrt{\left(\frac{2}{45\pi a_{0}^{7}}\right)} r^{2} e^{-r/a_{0}} - \sqrt{\left(\frac{2}{5\pi a_{0}^{3}}\right)} e^{-r/a_{0}}$$

is the required wavefunction.

Problem 4. Show that for a Simple Harmonic Oscillator we have:

$$\langle n \mid x \mid m \rangle \sqrt{\left(\frac{\hbar}{2m\omega}\right)} \left[\sqrt{(m+1)} \, \delta_n, \, _{m+1} + \sqrt{(m)} \, \delta_n, \, _{m-1}\right].$$

Hence evaluate the matrix elements for x^2 , x^3 and x^4 for the states of the simple harmonic oscillator.

Sol. The wavefunctions for a simple harmonic oscillator is given by

$$\frac{\psi_n(x)}{\sqrt{2^n n! \sqrt{n}}} e^{-\alpha^2 x^2/2} H_n(\alpha x); \alpha = \sqrt{\frac{m\omega}{\hbar}}, \dots (i)$$
where $H_n(\alpha x)$ is the Hermite polynomial of degree 'n'.

We have the following

We have the following recurrence relation for the Hermite polynomial H_n ,

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi).$$
 ...(ii)

Now, we can write the matrix element

$$\langle n \mid x \mid m \rangle = \int \psi_{n}^{*}(x) x \psi_{m}(x) dx$$

$$= \frac{\alpha}{\sqrt{(2^{n+m} \cdot n! m! \pi)}} \int e^{-\alpha^{2}x^{2}} H_{n}(\alpha x) x H_{m}(\alpha x) dx$$

$$= \frac{1}{\sqrt{(2^{n+m} \cdot n! m! \pi)}} \int e^{-\alpha^{2}x^{2}} H_{n}(\alpha x)$$

$$\times \left[\frac{1}{2} H_{m+1}(\alpha x) + m H_{m-1}(\alpha x) \right] dx \text{ {Using (ii)}} \right]$$

$$= \int \left(\frac{m+1}{2} \right) \cdot \frac{1}{\alpha} \int_{\Lambda} \left\{ \frac{\alpha}{2^{n} n! \sqrt{(\pi)}} \right\} e^{-\alpha^{2}x^{2}/2} H_{n}(\alpha x)$$

$$\times \sqrt{\left\{ \frac{\alpha}{2^{m+1} \cdot (m+1)! \sqrt{(\pi)}} \right\}} e^{-\alpha^{2}x^{2}/2} H_{m+1}(\alpha x) dx$$

$$+ \sqrt{\left\{ \frac{m}{2} \right\} \cdot \frac{1}{\alpha} \int_{\Lambda} \sqrt{\left\{ \frac{\alpha}{2^{n} n! \sqrt{(\pi)}} \right\}} e^{-\alpha^{2}x^{2}/2} H_{n}(\alpha x)$$

$$\times \sqrt{\left\{ \frac{\alpha}{2^{m-1} \cdot (m-1)! \sqrt{(\pi)}} \right\}} H_{m-1}(\alpha x) dx$$

$$= \sqrt{\left(\frac{m+1}{2} \right) \cdot \frac{1}{\alpha} \int_{\Lambda} \psi_{n}(x) \psi_{m+1}(x) dx}$$

$$+ \sqrt{\left(\frac{m}{2} \right) \cdot \frac{1}{\alpha} \int_{\Lambda} \psi_{n}(x) \psi_{m+1}(x) dx}$$

$$= \frac{1}{\sqrt{(2) \alpha}} \left[\sqrt{(m+1)} \delta_{n}, m+1} + \sqrt{(m)} \delta_{n}, m-1} \right],$$

or
$$\langle n \mid x \mid m \rangle = \sqrt{\left(\frac{\hbar}{2m\omega}\right)} \left[\sqrt{(m+1)} \delta_n, \frac{1}{m+1} + \sqrt{(m)} \delta_n, \frac{1}{m-1}\right] \dots (iii)$$

We can find the matrix elements of x^2 , x^3 and x^4 by the rule of multiplying the matrices. We have

$$\langle n \mid x^{2} \mid m \rangle = \sum_{t}^{\infty} \langle n \mid x \mid t \rangle \langle t \mid x \mid m \rangle$$

$$= \frac{\hbar}{2m\omega} \sum_{t}^{\infty} \left[\sqrt{(t+1)} \, \delta_{n}, \, _{t+1} + \sqrt{(t)} \, \delta_{n}, \, _{t-1} \right] \times \left[\sqrt{(m+1)} \, \delta_{t}, \, _{m+1} + \sqrt{(m)} \, \delta_{t}, \, _{m-1} \right]$$

$$= \frac{\hbar}{2m\omega} \left[\sqrt{\{(m+2) \, (m+1)\}} \, \delta_{n}, \, _{m+2} + m \, \delta_{n}, \, _{m} + (m+1) \, \delta_{n}, \, _{m} + \sqrt{\{(m+1) \, m\}} \, \delta_{n}, \, _{m-2} \right]$$

$$= \frac{\hbar}{2m\omega} \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m+2} \right. \\ + \sqrt{\{m\ (m-1)\}} \, \delta_{n,\ m-2} + (2m+1) \, \delta_{n,\ m} \right]. \dots (|v|)$$

$$\langle n \mid x^3 \mid m \rangle = \sum_{t} \langle n \mid x^2 \mid t \rangle \, \langle t \mid x \mid m \rangle$$

$$= \left(\frac{\hbar}{2m\omega} \right)^{3/2} \sum_{t} \left[\sqrt{\{(t+2)\ (t+1)\}} \, \delta_{n,\ t+2} \right. \\ + \sqrt{\{t\ (t-1)\}} \, \delta_{n,\ t-2} + (2t+1) \, \delta_{n,\ t]} \right. \\ \times \left[\sqrt{(m+1)} \, \delta_{t,\ m+1} + \sqrt{(m)} \, \delta_{t,\ m-1} \right]$$

$$= \left(\frac{\hbar}{2m\omega} \right)^{3/2} \left[\sqrt{\{(m+3)\ (m+2)\ (m+1)\}} \, \delta_{n,\ m+4} \right. \\ + \left. (m+1) \, \sqrt{(m)} \, \delta_{n,\ m-1} + (2m+3) \sqrt{(m+1)} \, \delta_{n,\ m+4} \right. \\ + \left. (m+1) \, \sqrt{(m)} \, \delta_{n,\ m-1} + (2m+3) \sqrt{(m+1)} \, \delta_{n,\ m+2} \right. \\ + \left. (2m-1) \, \sqrt{(m)} \, \delta_{n,\ m-1} \right]$$

$$= \left(\frac{\hbar}{2m\omega} \right)^{3/2} \left[\sqrt{\{(m+1)\ (m+2)\ (m+3)\}} \, \delta_{n,\ m+2} \right. \\ + \left. (3m+3) \, \sqrt{(m+1)} \, \delta_{n,\ m+1} + (2m-1) \sqrt{(m)} \, \delta_{n,\ m-1} \right. \\ + \left. \sqrt{\{m\ (m-1)\ (m-2)\}} \, \delta_{n,\ m-3} \right] \right. \\ \cdot \left. (n \mid x^4 \mid m \rangle = \sum_{t} \langle n \mid x^2 \mid t \rangle \, \langle t \mid x^2 \mid m \rangle$$

$$= \left(\frac{\hbar}{2m\omega} \right)^2 \sum_{t} \left[\sqrt{\{(t+1)\ (t+2)\}} \, \delta_{n,\ m+4} \right. \\ + \left. \sqrt{\{t\ (t-1)\}} \, \delta_{n,\ m+2} + (2t+1) \, \delta_{t,\ m} \right] \right. \\ = \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(t+1)\ (t+2)\}} \, \delta_{n,\ m+2} \right. \\ + \left. \sqrt{\{m\ (m-1)\}} \, \delta_{n,\ m+2} + (2m+1) \, \delta_{t,\ m} \right. \\ + \left. \sqrt{\{m\ (m-1)\}} \, \delta_{n,\ m+2} + (m-1) \, \delta_{n,\ m+4} \right. \\ + \left. \sqrt{\{m\ (m-1)\ (m-2)\ (m-3)\}} \, \delta_{n,\ m-2} \right. \\ + \left. (2m+1) \, \sqrt{\{m\ (m-1)\}} \, \delta_{n,\ m-2} + (2m+1)^2} \, \delta_{n,\ m+4} \right. \\ + \left. \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\ (m+2)\}} \, \delta_{n,\ m+2} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\ (m+3)\ (m+4)\}} \, \delta_{n,\ m+4} \right. \\ + \left. \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m-2} + (2m+1)^2} \, \delta_{n,\ m} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m-2} + (2m+1)^2} \, \delta_{n,\ m+4} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m+2} + (2m+1)^2} \, \delta_{n,\ m+4} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m+2} + (2m+1)^2} \, \delta_{n,\ m+4} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m+2} + (2m+1)^2} \, \delta_{n,\ m+4} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n,\ m+2} + (2m+1)^2} \, \delta_{n,\ m+4} \right. \\ + \left. \left(\frac{\hbar}{2m\omega} \right)^2 \left[\sqrt{\{(m+1)\ (m+2)\}} \, \delta_{n$$

Problem 5. For HCl molecule, the inter-nuclear distance is $1.29\text{Å}, m_{Ci}=35 m_H$ and $m_{H}=1.68\times 10^{-24} gm$. molecule as a rigid rotator, calculate the separation of the lines in the Considering the

Reduced mass of the molecule is given by:

$$\mu = \frac{m_H \cdot m_{Ci}}{m_H + m_{Ci}} = \frac{m_H \cdot 35m_H}{m_H + 35m_H} = \frac{35}{36} m_H$$

$$= \frac{35}{36} \cdot 1.68 \times 10^{-24} \text{ gms.} = 1.633 \times 10^{-24} \text{ gms.}$$

:. The moment of inertia of the molecule about the centre of mass is given by:

$$I = \mu r_0^2 = 1.633 \times 10^{-24} \times (1.29 \times 10^{-8})^2 \text{ gm. cm.}^2$$

 $\approx 2.722 \times 10^{-40} \text{ gm.-cm.}^2$

Considering the HCl molecule as a rigid rotator, its energy levels are given by:

$$E_l = \frac{\hbar^2}{2I} l (l+1) ; l=0, 1, 2, 3, \dots$$

Now, if the molecule goes from a higher energy level (l+1) to a lower level I, the energy of the radiation emitted is given by

$$E = E_{l+1} - E_l = \frac{\hbar^2}{2I} \left[(l+1) (l+2) - l (l+1) \right]$$

$$= \frac{\hbar^2}{2I} \cdot (l+1) \cdot 2 = \frac{\hbar^2}{I} (l+1) \text{ ergs.}$$

Hence, the wave-number of the spectral line corresponding to this energy is given by:

$$\bar{v} = \frac{E}{hc} = \frac{1}{hc} \cdot \frac{\hbar^2}{I} (l+1) = \frac{h}{4\pi^2 cI} (l+1) \text{ cm.}^{-1}.$$

Since $l=0, 1, 2, \ldots$ the lines in the spectrum are equidistant with a separation given by:

$$\frac{h}{4\pi^2 cI} = \frac{6.625 \times 10^{-27}}{4\pi^2 \cdot (3 \times 10^{10}) \cdot 2.722 \times 10^{-40}} \text{ cm.}^{-1}$$
$$= 20.68 \text{ cm}^{-1}.$$

7

ORBITAL AND SPIN ANGULAR MOMENTA

7.1. ORBITAL ANGULAR MOMENTUM:

In Classical Mechanics, the orbital angular momentum of a particle rotating about some axis is given by

$$L=r\times p,$$
 ...(1)

where r is the position vector from the axis of rotation and p is the linear momentum of the particle.

According to correspondence principle, the operator which represents angular momentum in quantum mechanics can be obtained from eqn. (1) by replacing p with its quantum mechanical operator $-i\hbar \nabla$,

$$\mathbf{L} = -i \, \mathbf{h} \mathbf{r} \times \nabla. \tag{2}$$

The three components of L can thus be written, in the cartesian coordinates as:

$$L_{x}=yp_{z}-zp_{y}=-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)$$

$$L_{y}=zp_{x}-xp_{z}=-i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right),$$

$$L_{z}=xp_{y}-yp_{x}=-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right).$$
(3)

In order to represent these in the spherical polar co-ordinates, we use the relations

$$x = r \sin \theta \cos \phi,$$

$$y = r \sin \theta \sin \phi,$$

$$z = r \cos \theta,$$
...(4)

between the cartesian and the polar co-ordinates. We have from (4) that

$$r = (x^2 + y^2 + z^2)^{1/2}$$
; $\tan \theta = \frac{\sqrt{(x^2 + y^2)}}{z}$ and $\tan \phi = \frac{y}{x}$
$$\frac{\partial r}{\partial x} = \sin \theta \cos \phi, \frac{\partial r}{\partial y} = \sin \theta \sin \phi; \frac{\partial r}{\partial z} = \cos \theta;$$

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$$\frac{\partial \theta}{\partial x} = \frac{\cos \theta \cos \phi}{r}; \frac{\partial \theta}{\partial y} = \frac{\cos \theta \sin \phi}{r}; \frac{\partial \theta}{\partial z} = 0;$$

$$\frac{\partial \phi}{\partial x} = -\frac{\sin \phi}{r \sin \theta}; \frac{\partial \phi}{\partial y} = \frac{\cos \phi}{r \sin \theta}$$

$$\therefore \frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial r} \cdot \frac{\partial r}{\partial x} + \frac{\partial \psi}{\partial \theta} \cdot \frac{\partial \theta}{\partial x} + \frac{\partial \psi}{\partial \phi} \cdot \frac{\partial \phi}{\partial x}$$

$$= \sin \theta \cos \phi \frac{\partial \psi}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial \psi}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial \psi}{\partial \phi}$$

$$\Rightarrow \frac{\partial}{\partial x} = \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$\therefore (5a)$$

Similarly,
$$\frac{\partial}{\partial y} = \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \dots (5b)$$

and

$$\frac{\partial}{\partial z} = \cos \theta \, \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \, \frac{\partial}{\partial \theta}. \qquad ...(5c)$$

Using equations (4) and (5) into eqns. (3) we get

equations (4) and (5)
$$L_{x}=-i\hbar\left(-\cot\theta\cos\phi\,\frac{\partial}{\partial\phi}-\sin\phi\,\frac{\partial}{\partial\theta}\right),$$

$$L_{y}=-i\hbar\left(-\cot\theta\sin\phi\,\frac{\partial}{\partial\phi}+\cos\phi\,\frac{\partial}{\partial\theta}\right),$$

$$L_{z}=-i\hbar\,\frac{\partial}{\partial\phi}.$$

$$L_{z}=-i\hbar\,\frac{\partial}{\partial\phi}.$$
This defined as

Square of the angular momentum L is defined as

$$L^{2} = L_{x}^{2} + L_{y}^{2} + L_{z}^{2}$$

$$= -\hbar^{2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} \right]. \quad ...(7)$$

COMMUTATION RELATIONS FOR ORBITAL ANGU-7.2. LAR MOMENTUM:

Various commutation relations between the components of L and L2 can be derived by using the fundamental commutation relations between the components of r and p. For example

$$[L_x, y] = [yp_z - zp_y, y] = [yp_z, y] - [zp_y, y]$$

$$= y [p_z, y] + [y, y] p_z - z [p_y, y] - [z, y] p_y$$

$$= y \cdot 0 + 0 \cdot p_z - z \cdot \bullet i\hbar - 0 \cdot p_y = i\hbar z.$$

Similarly, $[L_x, x] = 0$ and $[L_x, z] = -i\hbar y$.

Similar relations for other components of L can be written by a cyclic permutation of the indices x, y and z.

Further, we can also derive the relation

$$[L_{x}, p_{y}] = [yp_{z} - zp_{y}, p_{y}] = [yp_{z}, p_{y}] - [zp_{y}, p_{y}]$$

$$= y [p_{z}, p_{y}] + [y, p_{y}] p_{z} - z [p_{y}, p_{y}] - [z, p_{y}] \cdot p_{y}$$

$$= y \cdot 0 + i \ln p_{z} - z \cdot 0 - 0 \cdot p_{y} = i \ln p_{z}.$$

Similarly, $[L_x, p_x] = 0$ and $[L_x, p_x] = -i\hbar p_y$,

with similar relations for the other components of L, which can be obtained by a cyclic permutation of the indices x, y and z.

Using the above commutation relations, we can deduce the commutation relations between the various components of L as

$$[L_x, L_y] = [L_x, zp_x - xp_z] = [L_x, z] p_x - x [L_x, p_z]$$

$$= -i\hbar y p_x + i\hbar x p_y = i\hbar L_z.$$

Similarly, $[L_x, L_x] = 0$; $[L_x, L_z] = -i\hbar L_y$; $[L_y, L_z] = i\hbar L_x$ etc. Also, we have

$$[L^{2}, L_{z}] = [L_{x}^{2} + L_{y}^{2} + L_{z}^{2}, L_{z}] = [L_{x}^{2} + L_{y}^{2}, L_{z}]$$

$$\{ :: L_{z} \text{ commutes with } L_{z}^{2} \}$$

$$= L_{x} [L_{x}, L_{z}] + [L_{x}, L_{z}] L_{x} + L_{y} [L_{y}, L_{z}] + [L_{y}, L_{z}] L_{y}$$

$$= -i \hbar L_{x} L_{y} - i \hbar L_{y} L_{z} + i \hbar L_{y} L_{x} + i \hbar L_{x} L_{y}$$

$$= 0$$

Similarly,

$$[L^2, L_x] = [L^2, L_y] = 0.$$

Therefore, in general

$$[L^2, L] = 0.$$

From above relations we see that no two components of L commutes, the system cannot in general be assigned definite values for all angular momentum components, due to the uncertainty principle. On the other hand it is possible to measure simultaneously and precisely the value of L^2 and the components of L and hence L2 and L.

7.3. EIGEN-VALUE PROBLEM FOR L2:

The eigenvalue equation for L2 can be written as

$$L^2\psi = \lambda\psi,$$
 ...(8)

where ψ is the eigenfunction of L^2 with an eigenvalue λ .

Using eqn. (7), it can be written as

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} = -\frac{\lambda}{\hbar^2} \psi. \tag{9}$$

To solve this differential equation we use the separation of variables method and write ...(10)

$$\psi = \Theta (\theta) \Phi (\phi). \qquad \dots (10)$$

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Substituting eq. (10) in (9) and dividing throughout by ψ , we get

$$\frac{1}{\Theta} \cdot \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi} \cdot \frac{1}{\sin^2 \theta} \cdot \frac{\partial^2 \Phi}{\partial \phi^2} = -\frac{\lambda}{\hbar^2}$$

$$-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = \frac{\sin^2\theta}{\Theta} \left[\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) + \frac{\lambda}{\hbar^2} \right]. \quad \dots (11)$$

The left hand side of the above equation is independent of θ while the right hand side is independent of ϕ . Thus the derivative of L.H.S. w.r.t. θ vanishes and hence the L.H.S. is a constant independent of θ . Similarly the R.H.S. is a constant independent of ϕ . The equality of the two sides shows that they have a common constant value independent of θ and ϕ . Denoting it by m^2 , we can write equation (11) as two equations

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0 \qquad \dots (12a)$$

and

i.e.

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) - \frac{m^2}{\sin^2 \theta} \Theta + \frac{\lambda}{\hbar^2} \Theta = 0. \quad \dots (12b)$$

Solution of (12a) is seen to be

$$\Phi (\phi) = C_1 e^{\pm im\phi}, \qquad .. (13)$$

where C_1 is the constant of integration.

Now, the physically meaningful wavefunctions in quantum mechanics are the functions which are finite, single valued and the derivatives of which are continuous. Since values of ϕ differing by integral multiples of 2π refer to the same point in space, solutions (13) will satisfy the condition of single-valuedness only if $e^{\pm im\phi} = e^{\pm im(\phi + 2\pi)}$,

$$e^{\pm im\phi} = e^{\pm im(\phi + 2\pi)},$$

 $e^{2\pi im} = 1 \Rightarrow m = 0, \pm 1, \pm 2, ...$

Thus m will be an integer, positive or negative, and the physical solutions of (12a) are

$$\Phi(\phi) = C_1 e^{im\phi}, m = 0, \pm 1, \pm 2, \dots$$
 ...(14)

Note that since both signs of m are included it is not necessary to mention $e^{-im\phi}$ separately.

The constant C_1 can be chosen to normalize Φ as:

i.e.
$$\int_{0}^{2\pi} \Phi^* \Phi \ d\phi = 1$$
$$|C_1|^2 \int_{0}^{2\pi} d\phi = 1$$
or
$$|C_1|^2 . 2\pi = 1 \Rightarrow C_1 = (2\pi)^{-1/2}$$

Hence the normalized solution of eqn. (12-a) is given by

$$\Phi(\phi) = (2\pi)^{-1/2} e^{im\phi}; m=0, \pm 1, \pm 2, \dots$$
 ...(15)

To solve (12-b), we substitute $\mu = \cos \theta$ in it, we get

$$\frac{d}{d\mu} \left\{ (1-\mu^2) \frac{d\Theta}{d\mu} \right\} + \left(\frac{\lambda}{\hbar^2} - \frac{m^2}{1-\mu^2} \right) \Theta = 0$$

or
$$(1-\mu^2) \frac{d^2\Theta}{d\mu^2} - 2\mu \frac{d\Theta}{d\mu} + \left(\frac{\lambda}{\hbar^2} - \frac{m^2}{1-\mu^2}\right) \Theta = 0$$
 ...(16)

For the special case m=0, eqn. (16) assumes the form

$$(1-\mu^2)\frac{d^2\Theta}{d\mu^2} - 2\mu \frac{d\Theta}{d\mu} + \left(\frac{\lambda}{\hbar^2}\right)\Theta = 0 \qquad \dots (17)$$

To find the solution of eqn. (17), we write a power series for Θ ,

$$\Theta = \sum_{k=0}^{\infty} C_k \mu^k \qquad \dots (18)$$

Substituting it into eqn. (17) and comparing the co-efficients of μ^k , we get the following recursion relation for the coefficients C_k

$$C_{k+2} = \frac{k (k+1) - \lambda/\hbar^2}{(k+1) (k+2)} C_k \qquad ...(19)$$

For very large values of k, we have from eqn. (19) that

$$\frac{C_{k+2}}{C_k} \to \frac{k}{k+2}$$

This ratio permits the conclusion that for large values of k; Θ behaves like the series $\sum_{0}^{\infty} \mu^{j_{c}}/k$, because the ratio of consecutive coefficients in this series is also k/(k+2). For $\mu=\pm 1$ i.e. $\theta=0$, π , the series $\sum_{0}^{\infty} \mu^{j_{c}}/k$ diverges. Thus Θ and hence ψ is not finite and cannot be admitted as an eigenfunction of L^{2} . The only way in which this situation can be avoided is to choose λ in such a way that the power series for Θ is cut off after some finite number of terms, making Θ a polynomial. Let us suppose that the power series terminates at some finite value of k=l (say), where l is a positive integer, and all higher powers vanish. According to eqn. (19), it will be so if λ has the value given by

$$\lambda = \hbar^2 l (l+1) \qquad \dots (20)$$

These are the eigenvalues of L^2 for l=0, 1, 2, ...l is known as the orbital angular momentum quantum number.

Using eqn. (20), we can write equation (17) as:

$$(1-\mu^2)\frac{d^2\Theta}{d\mu^2} - 2\mu \frac{d\Theta}{d\mu} + l(l+1)\Theta = 0 \qquad ...(21)$$

This is the well known Legendre's equation and its solution is the Legendre's polynomial of degree l:

$$\Theta = P_{l}(\mu) = \frac{1}{l! \ 2^{l}} \frac{d^{l}(\mu^{2} - 1)^{l}}{d\mu^{l}} \qquad ...(22)$$

Thus we have solved equation (16) for the special case where m=0. Now we can find the solution for the case $m\neq 0$ by using the solution for m=0. For it we differentiate equation (17) m=0 times (using Lebniz's rule) and write $\frac{d^m\Theta}{d\mu^m}=v$, we get

$$(1-\mu^2) \frac{d^2v}{d\mu^2} - 2\mu (m+1) \frac{dv}{d\mu} + (l-m) (l+m+1) v = 0. \qquad ...(23)$$

Since $P_i(\mu)$ is a solution of eqn. (17); equation (23) is satisfied by

$$v = \frac{d^m P_l(\mu)}{d\mu^m}.$$
 ...(24)

If we substitute w=v $(1-\mu^2)^{m/2}$ in eqn. (23), we get

$$(1-\mu^2) \frac{d^2w}{d\mu^2} - 2\mu \frac{dw}{d\mu} + \left(l(l+1) - \frac{m^2}{1-\mu^2}\right) w = 0. \tag{25}$$

This is identical to the equation (27) for $\lambda = \hbar^2 l(l+1)$ and is known as the associated Legendre's equation. From it we see that solution of eqn. (16) is given by:

$$\Theta(\theta) = w = P_l^m (\mu) = (1 - \mu^2)^{m/2} \frac{d^m P_l(\mu)}{d\mu^m} \dots (26)$$

Here $w=P_l^m(\mu)$ are called the associated Legendre's polynomials and these are defined for positive integers $m \leq l$. These are the only physically acceptable solutions of eqn. (16). To normalize Θ , we write

$$|C|^2 \int_{-1}^{+1} P_i^m (\cos \theta) P_i^m (\cos \theta) d \cos \theta = 1.$$

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$$|C|^2 \frac{2}{2l+1} \cdot \frac{(l+m)!}{(l-m)!} = 1$$

{Using the orthogonality relation for P_1^m ;

$$\Rightarrow C = \sqrt{\left(\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m)!}\right)}$$

Therefore, normalized Θ is given by

$$\Theta = \sqrt{\left(\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m)!}\right)} P_{l}^{m} \left(\cos \theta\right) \qquad \dots (27)$$

Hence the normalized eigenfunctions of L2 can be written as:

$$\psi = Y_l^m(\theta, \phi) = \theta(\theta) \Phi(\phi) = \epsilon \left[\frac{2l+1}{4\pi} \cdot \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\cos\theta) e^{im\phi}$$

Here $\psi = Y_I^m(\theta, \phi)$ are called the spherical Harmonics, ϵ is a phase factor, chosen for later convenience as $\epsilon = (-1)^m$ for $m \ge 0$ and $\epsilon = 1$ for m < 0.

7.4. EIGEN VALUE PROBLEM FOR L_z , L_y and L_z :

We have seen that L^2 commutes with all the three components of L. Therefore it is possible to construct the simultaneous eigenfunctions for L^2 and a component of L. We note that

$$L_{z} Y_{l}^{m} (\theta, \phi) = -i \hbar \frac{\partial}{\partial \phi} Y_{l}^{m} (\theta, \phi) = \hbar m Y_{l}^{m} (\theta, \phi) \qquad ...(29)$$

i.e. $Y_l^m(\theta, \phi)$ is the eigenfunction of L_z with an eigenvalue hm where m is any integer, positive or negative The number m is known as the magnetic quantum number.

Thus the spherical harmonics are the normalized simultaneous eigenfunctions of L_z and L^2 .

In order to find the effect of L_x and L_y on Y_l^m (θ, ϕ) we define two operators L_+ and L_- as:

$$L_{+}=L_{x}+iL_{y}$$
; $L_{-}=L_{x}-iL_{y}$(30)

It is eary to verify the following properties of these operators,

$$L_{+}^{*}=L_{-}$$

$$L_{+}L_{-}=L^{2}-L_{z}^{2}+\hbar L_{z}$$

$$L_{-}L_{+}=L^{2}-L_{z}^{2}-\hbar L_{z}$$

$$[L_{+}, L_{z}]=-\hbar L_{+}$$

$$[L_{-}, L_{z}]=\hbar L_{-}$$

$$[L_{+}, L_{-}]=2\hbar L_{z}$$

According to eqns. (6), we have

$$L_{+} = \hbar e^{i\phi} \left(\frac{\partial}{\partial \theta} + i \cos \theta \frac{\partial}{\partial \phi} \right)$$

$$L_{-} = -\hbar e^{-i\phi} \left(\frac{\partial}{\partial \theta} - i \cos \theta \frac{\partial}{\partial \phi} \right)$$
...(31)

The effect of $\frac{\partial}{\partial \phi}$ on $Y_{l}^{m}(\theta, \phi)$ is known. To determine the

effect of $\frac{\partial}{\partial \theta}$ we note that from the definition, eqn. (26)

$$\frac{dP_l^m}{d\mu} = \frac{1}{\sqrt{(1-\mu^2)}} \cdot P_l^{m+1} - \frac{m\mu}{1-\mu^2} \rho_l^m$$

With $\mu = \cos \theta$ and the definition eqn. (28) it is easily seen that

$$L_{+}Y_{l}^{m}(\theta, \phi) = \hbar \sqrt{\{(l-m)(l+m+1)\}} Y_{l}^{m+1}(\theta, \phi)$$

$$L_{-}Y_{l}^{m}(\theta, \phi) = \hbar \{(l+m)(l-m+1)\} Y_{l}^{m-1}(\theta, \phi)$$
Using these relations we see that
$$L_{x}Y_{l}^{m}(\theta, \phi) = \frac{1}{2} (L_{+} + L_{-}) Y_{l}^{m}(\theta, \phi)$$

$$= \frac{\hbar}{2} \sqrt{\{(l-m)(l+m+1)\}} Y_{l}^{m+1}(\theta, \phi)$$

$$+ \frac{\hbar}{2} \sqrt{\{(l+m)(l-m+1)\}} Y_{l}^{m-1}(\theta, \phi) \dots (33a)$$
and
$$L_{y}Y_{l}^{m}(\theta, \phi) = \frac{1}{2i} (L_{+} - L_{-}) Y_{l}^{m}(\theta, \phi)$$

$$= \frac{\hbar}{2i} \sqrt{\{(l-m)(l+m+1)\}} Y_{l}^{m+1}(\theta, \phi)$$

$$- \frac{\hbar}{2i} \sqrt{\{(l+m)(l-m+1)\}} Y_{l}^{m-1}(\theta, \phi) \dots (33b)$$

Thus $Y_l^m(\theta, \phi)$ are not the simultaneous eigenfunctions of L^2 and L_x or L_y . But we can construct new functions by using the method of section 11 of Chapter -2 on Operators in Quantum Mechanics using Y_l^m for various values of m. The procedure is quite involved and cumbersome and hence we omit that here.

7.5. MATRIX ELEMENTS OF ORBITAL ANGULAR MOMENTUM OPERATORS:

The spherical harmonics satisfy the following orthonormality relation

$$\int_{0}^{2\pi} \int_{0}^{\pi} Y_{l}^{m*}(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \sin \theta \, d\theta \, a\phi = \delta_{ll'} \delta_{mm'} \qquad \dots (34)$$

Using this we can write down the matrix elements for L^2 and L_z as

$$(L^{2})_{l, l'; m, m'} = \int_{0}^{2\pi} \int_{0}^{\pi} Y_{l}^{m^{*}}(\theta, \phi) L^{2} Y_{l'}^{m'}(\theta, \phi) \sin \theta d\theta d\phi$$

$$= \hbar^{2} l' (l'+1) \delta_{ll'} \delta_{mm'} \qquad ...(35)$$

$$(L_{z})_{l, l'; m, m'} = \int_{0}^{2\pi} \int_{0}^{\pi} Y_{l}^{m^{*}}(\theta, \phi) L_{z} Y_{l'}^{m'}(\theta, \phi) \sin \theta \, d\theta \, d\phi$$

$$= \hbar m' \, \delta_{ll'} \, \delta_{mm'} \qquad ...(36)$$

There remains the problem of obtaining the matrix elements for L_x and L_y . To do this, we work in terms of the operators L_+ and L_- . Using eqn. (32) we have

$$(L_{+})_{l, l'; m, m'} = (L_{x} + i L_{y})_{l, l'; m, m'}$$

$$= \int_{0}^{2\pi} \int_{0}^{\pi} Y_{l}^{m} (\theta, \phi) L_{+} Y_{l'}^{m'} (\theta, \phi) \sin \theta \, d\theta \, d\phi$$

$$= \hbar \sqrt{\{(l'-m') (l'+m'+1) \delta_{l, l'} \delta_{m, m'+1} \dots (37) \}}$$

and
$$(L_{-})_{l, l'; m, m'} = (L_{x} - i L_{y})_{l, l'; m, m'}$$

$$= \int_{0}^{2\pi} \int_{0}^{\pi} Y_{l}^{m} (\theta, \phi) L_{-} Y_{l'}^{m'} (\theta, \phi) \sin \theta \, d\theta \, d\phi$$

$$= \hbar \sqrt{\{l' + m'\} (l' - m' + 1) \delta_{l, l'} \delta_{m, m'} - 1.} \dots (38)$$

From eqn. (37) and (38) we see that $(L_x+i L_y)$ and $(L_x-i L_y)$ are represented by matrices which are diagonal in l, but in which all elements are one position off the diagonal in m.

Now for a particular value of l, m can have (2l+1) values, $m=0, \pm 1, \pm 2, \ldots, \pm l$. Thus the angular momentum matrices for a given value of l will be a (2l+1) dimensional representation. A few of these for different values of l are written below explicitly:

For.
$$l=2$$
.

7.6. SPIN ANGULAR MOMENTUM:

The magnetic moment m of an electron circulating in an orbit with an orbital angular momentum L is given by

$$\mathbf{m} = -\frac{e}{2mc} \mathbf{L}, \qquad \dots (39)$$

where m is the mass and e the charge of the electron.

In quantum mechanics each component of L has (2l+1) eigenvalues e.g. L_z has values from -l to +l. Since l is an integer, (2l+1) will be an odd number. These odd number of states have the same energy and the orbital angular momentum. When a weak magnetic field is applied there should occur a splitting of these degenerate levels.

Stern-Gerlach performed an experiment in which they passed a beam of silver atoms through an inhomogeneous magnetic field. They obtained only two (an even number) of traces on a screen. If we suppose that the single valence electron in silver atom outside the spherically symmetric closed shell should be in its lowest energy state (l=0), we should get only one trace according to eqn. (39).

In order to resolve this difficulty, Uhlenbeck and Goudsmit proposed that in addition to the orbital angular momentum L,

each electron has some intrinsic angular momentum S, called the spin angular momentum. There is associated a spin magnetic

moment $\overrightarrow{\mu}$ with this spin angular momentum

$$\overrightarrow{\mu} = -\frac{e}{mc} \mathbf{S} \qquad \dots (40)$$

The value of the spin angular momentum for the electron was assigned to be $\frac{1}{2}\hbar$, which has two components $\pm \frac{1}{2}\hbar$ in any direction, so that in particular

 $S_z = \pm \frac{1}{2}\hbar$

Thus each orbital electron provides a contribution of $\frac{\pm e\hbar}{2mc}$ to the angular momentum in an assigned direction. The two projections in the Stern-Gerlach experiment can now be associated with these two components of the spin magnetic moment.

The spin angular momentum is not the attribute of the electrons only, but all quantum mechanical systems are assigned with a value of it. It is found experimentally that electrons, protons, neutrons, neutrinos, and μ -mesons each have a value $\frac{1}{2}\hbar$, photons, have ħ, and π-mesons have zero value of the spin angular momentum. Similarly, all the other particles and the quantum mechanical systems (aggregates of particles) can be characterized by a definite value of the spin angular momentum. Spin has no classical analogue and is introduced in non-relativistic quantum theory adhoc. [We shall see that the relativistic theory will itself endows the electron with a spin angular momentum]. The exercise of assigning it to some sort of rotation of the particle about its axis proved futile, because when we consider a complex system such as the nucleus, as a whole, we can talk of its total intrinsic angular momentum which we call the spin angular momentum of the nucleus, but strictly speaking there is nothing like spining of the nucleus. As the spin angular momentum cannot be attributed to any sort of spin or orbital motion, it is independent of r and p. Thus the definition (2) of the otbital angular momentum L, cannot be applied to the spin angular momentum. We now go ahead and generalize the definition of the angular momentum as a Hermitian operator whose components satisfy all the commutation relations satisfied by L^2 , L and its components (see section 7.2). Thus the spin angular momentum is an observable represented by an operator S with three components S_x , S_y and S_z which satisfies the following commutation relations:

$$[S_x, S_y] = i \hbar S_z$$

$$[S_y, S_z] = i \hbar S_x$$

$$[S_z, S_x] = i \hbar S_y$$
...(41)

and

Defining

$$S_{+} = S_{x} + iS_{y}$$

$$S_{-} = S_{x} - iS_{y}$$

$$S^{2} = S_{x}^{2} + S_{y}^{2} + S_{z}^{2}$$
...(42)

and

we can very easily derive the following commutation relations using the relations of eqn. (41).

$$[S_{+}, S_{z}] = -\hbar S_{+}; [S_{-}, S_{z}] = \hbar S_{-}$$

$$[S_{+}, S_{-}] = 2\hbar S_{z}; S_{+}S_{-} = S^{2} - S_{z}^{2} + \hbar S_{z}$$

$$[S^{2}, S_{x}] = [S^{2}, S_{y}] = [S^{2}, S_{z}] = 0$$
...(43)

As the spin is an observable independent of the position and momentum coordinates, it commutes with position and momentum components and therefore, with the orbital angular momentum components also.

If ψ (spin) is the simultaneous eigenfunction of S^2 and S_z , then we have the following eigenvalue equations:

$$S^{2} \psi (\operatorname{spin}) = s (s+1) \hbar^{2} \psi (\operatorname{spin})$$

$$S_{z} \psi (\operatorname{spin}) = s_{z} \hbar \psi (\operatorname{spin})$$

$$\dots(44)$$

Here s is known as the spin quantum number, and it can have integral as well as half integral values, but exclusively one or the other for a given type of particle. s_z is the z-component of the spin and can have values from -s to +s in integral steps: i.e., -s, -s+1, ..., 0, 1, 2, ..., s. The spin wavefunction ψ (spin) can be designated by the values s and s_z with the following orthonormality relation:

Using this relation we can write the matrix elements for the various spin operators for a particular value of the spin quantum number s. As an explicit example, the matrices for an electron with $s=\frac{1}{2}$ are written below:

$$\frac{S_{z}}{\hbar} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}; S_{+}/\hbar = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; S_{-}/\hbar = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix};$$
Hence,
$$\frac{S_{x}}{\hbar} = \frac{1}{2\hbar} (S_{+} + S_{-}) = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix};$$

$$\frac{S_{y}}{\hbar} = \frac{1}{2i\hbar} (S_{+} - 1) = \begin{pmatrix} 0 & -i/2 \\ i/2 & 0 \end{pmatrix};$$

and

$$S^{2} = S_{x}^{2} + S_{y}^{2} + S_{z}^{2} = \begin{pmatrix} \frac{3}{4} & 0\\ 0 & \frac{3}{4} \end{pmatrix}$$

The corresponding wave function for the electron in matrix form can be represented as:

$$\psi \text{ (spin)} = \begin{pmatrix} \psi_{+} & (\mathbf{r}) \\ \psi_{-} & (\mathbf{r}) \end{pmatrix}; \text{ say} \qquad \dots (46)$$

Such a two component column representation is called a spinor.

For later convenience we write

$$S = \frac{1}{2} \hbar \sigma \qquad ...(47)$$

so ehat the eigenvalues of σ_x , σ_y , σ_z are simply ± 1 . The matrices

for the components of σ are explicitly given by

aponents of
$$\sigma$$
 are explicitly given by
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \dots (48)$$

The following These are called the Pauli Spin Matrices. relations can very easily be verified for these matrices.

an very easily be verified for these ... (49-a)
$$\sigma_{x}^{2} = \sigma_{y}^{2} = \sigma_{z}^{2} = I$$

$$\begin{array}{ccc}
\sigma_{x}\sigma_{y} - \sigma_{y}\sigma_{z} = 2i\sigma_{z} \\
\sigma_{y}\sigma_{z} - \sigma_{z}\sigma_{y} = 2i\sigma_{x} \\
\sigma_{z}\sigma_{x} - \sigma_{x}\sigma_{z} = 2i\sigma_{y}
\end{array}$$
or
$$\begin{array}{c}
\rightarrow & \rightarrow \\
\sigma_{x}\sigma_{z}\sigma_{x} - \sigma_{z}\sigma_{z} = 2i\sigma_{y}
\end{array}$$

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$$\sigma_{z}\sigma_{x} - \sigma_{x}\sigma_{z} = 2i\sigma_{y}$$

$$\sigma_{x}\sigma_{y} + \sigma_{y}\sigma_{x} = \sigma_{y}\sigma_{z} + \sigma_{z}\sigma_{y} = \sigma_{z}\sigma_{x} + \sigma_{x}\sigma_{z} = 0$$

$$(49)$$

$$\sigma_{x}\sigma_{y} + \sigma_{y}\sigma_{x} = \sigma_{y}\sigma_{z} + \sigma_{z}\sigma_{y} = \sigma_{z}\sigma_{x} + \sigma_{x}\sigma_{z}$$

$$\sigma_{x}\sigma_{y} = i \sigma_{z} ; \sigma_{y}\sigma_{z} = i \sigma_{x} ; \sigma_{z}\sigma_{x} = i \sigma_{y}$$
...(49-

GENERALIZED ANGULAR MOMENTUM:

As we have remarked in the last section that the definition $L=r\times p$ of the angular momentum cannot admit $\frac{1}{2}\hbar$ as a possible value. We, therefore, defined the angular momentum as an operator satisfying very general commutation relations, with those of L_x , L_y , L_z as a special case. In order to have a convenient notation for later work, we define a general angular momentum vector by the symbol J, with the components J_x , J_y , J_z ; satisfying the commutation relations:

mmutation relations.
$$[J_x, J_y] = i\hbar J_z; [J_y, J_z] = i\hbar J_x; [J_z, J_x] = i\hbar J_y \qquad ...(50)$$

$$[J_x, J_y] = i\hbar J_z; [J_y, J_z] = i\hbar J_x; [J_z, J_x] = i\hbar J_y \qquad ...(50)$$

J may be in particular, the orbital angular momentum L, tl spin angular momentum S or a combination of both.

Defining the operators $J_{+}=J_{x}\pm i\,J_{y}$ and $J^{2}=J_{x}^{2}+J_{y}^{2}+$ we can also show by using eqn. (50) that:

$$[J_{z}, J_{+}] = \hbar J_{+}; [J_{z}, J_{-}] = -\hbar J_{-};$$

$$[J^{2}, J_{w}] = [J^{2}, J_{y}] = [J^{2}, J_{z}] = 0;$$

$$J_{+}J_{-} = J^{2} - J_{z}^{2} + \hbar J_{z}; J_{-}J_{+} = J^{2} - J_{z}^{2} - \hbar J_{z};$$
and $[J_{+}, J_{-}] = 2\hbar J_{z}.$
...(51)

It can be shown immediately that Eqns. (50) and (51) are, by themselves, sufficient to determine the eigenvalue spectrum of J^2 as well as that of any component of J, and that the spectrum includes half integral values also.

7.8. THE EIGENVALUE SPECTRUM FOR J^2 AND J_z .

If we denote the eigenvalue of J_z by mh and that of J^2 by λh^2 , the simultaneous state-vector of J^2 and J_z can conveniently be written in ket notation as $|\lambda m\rangle$ and the eigenvalue equations can be written as:

$$J^{2} \mid \lambda m \rangle = \lambda \hat{\mathbf{n}}^{2} \mid \lambda m \rangle \qquad \dots (52-a)$$

$$J_{z} \mid \lambda m \rangle = m \hat{\mathbf{n}} \mid \lambda m \rangle \qquad \dots (52-b)$$

Now we show that the eigenvalues λ and m satisfy the inequality $\lambda \ge m^2$. For it we have,

$$J^{2}-J_{z}^{2}=\frac{1}{2}\left(J_{+}J_{-}+J_{-}J_{+}\right)$$

$$\therefore \langle \lambda m \mid J^{2}-J_{z}^{2} \mid \lambda m \rangle = \frac{1}{2}\langle \lambda m \mid J_{+}J_{-}+J_{-}J_{+} \mid \lambda m \rangle$$
or
$$(\lambda - m^{2}) \ \hbar^{2} \langle \lambda m \mid \lambda m \rangle = \frac{1}{2}\langle \lambda m \mid J_{+}J_{-}\dagger \mid \lambda m \rangle$$

$$+ \frac{1}{2}\langle \lambda m \mid J_{-}J_{-}\dagger \mid \lambda m \rangle \quad \{\because \quad J_{+}=J_{-}\dagger \text{ by definition}\}$$

$$= \frac{1}{2}\langle J_{+}\dagger \mid \lambda m \mid J_{+}\dagger \lambda m \rangle + \frac{1}{2}\langle J_{-}\dagger \lambda m \mid J_{-}\dagger \lambda m \rangle \geqslant 0.$$

$$\Rightarrow \lambda \geqslant m^{2} \qquad \dots (53)$$

Next we consider the operation of J_zJ_+ on $|\lambda m\rangle$. We have $J_zJ_+ |\lambda m\rangle = (\hbar J_+ + J_+J_\alpha) |\lambda m\rangle$ {Using $[J_z, J_+] = \hbar J_+$ } = $\hbar (m+1) J_+ |\lambda m\rangle$...(54-a)

Similarly,

$$J_z J_- |\lambda m\rangle = \ln (m-1) J_- |\lambda m\rangle$$
 ...(54-b)

Eqns. (54) show that $J_{+} \mid \lambda m \rangle$ are also eigenkets of J_{z} with eigenvalues $(m\pm 1)$ h. We may, therefore write that

and
$$J_{+} \mid \lambda m \rangle = C_{+} \mid \lambda, m+1 \rangle$$
$$J_{-} \mid \lambda m \rangle = C_{-} \mid \lambda, m-1 \rangle$$
$$\dots(55)$$

 C_+ and C_- are the proportionality constants and can be determined by the normality condition of $J_+ \mid \lambda m \rangle$. For a given value of λ , the inequality (53) limits the magnitude of m. If j is the greatest value of m for any given λ , application of the raising operator J_+ to the eigenket $\mid \lambda j \rangle$ should not lead to a new eigenket. Therefore,

$$J_+ \mid \lambda j \rangle = 0$$

- 1

Multiplying from left by J_{-} , we obtain

or
$$J_{+} | \lambda j \rangle = 0$$

$$(J^{2} - J_{z}^{2} - \hbar J_{z}) | \lambda j \rangle = 0$$
or
$$(\lambda - j^{2} - j) \hbar | \lambda j \rangle = 0$$
or
$$\lambda^{2} - j^{2} - j = 0 \text{ or } \lambda = j (j+1) \qquad \dots (56-a)$$

Similarly, if j' is the lowest value of m, then

$$J_{-} \mid \lambda j' \rangle = 0$$

operating on it from left by J_+ we can deduce that

$$\lambda = j'(j'-1)$$
 ...(56-b)

Equations (56-a) and (56-b) give j'(j'-1)=j(j+1)

$$j'(j'-1)=J(J+1)$$

 $\Rightarrow j'=-j \text{ or } j'=j+1.$

The second solution is meaningless because j is the greatest Hence j' = -j. value of m.

Since the eigenvalues have both the upper as well as lower bounds, it is obvious that for a given value of λ , or j, it must be possible to reach $|\lambda j'\rangle \equiv |\lambda, -j\rangle$ from $|\lambda j\rangle$ in a sufficient number of steps, descending the ladder by application of the lowering operator J_{-} . In each downward step, m decreases by unity. It follows that j-j'=2j must be a non-negative integer. Hence, j must be either a non-negative integer or a half-integer, i.e., the only possible values of j are

$$j=0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$$
 ... (57)

The corresponding values of $\lambda = j(j+1)$ are

$$\lambda = 0, \frac{3}{4}, 2, \frac{15}{4}, 6, \dots$$
 (58)

For a given value of j, the eigenvalues of J_z are $m\hbar = j\hbar$, $(j-1)\hbar$, $(j-2)\hbar$, ..., $0, ..., -(j-1)\hbar$, $-j\hbar$...(59)

These are (2j+1) in number.

We now determine the constants C_{\pm} of eqns. (55). We have $\langle \lambda m \mid J_{-} = \langle \lambda, m+1 \mid C_{+}^{*}$

$$\therefore \langle \lambda m \mid J_{-}J_{+} \mid \lambda m \rangle = |C_{+}|^{2} \langle \lambda, m+1 \mid \lambda, m+1 \rangle$$

Now assuming that the eigenvectors $|\lambda m\rangle$ are normalized to unity, we can write the above eqn. as:

or
$$[j(j+1)-m^2-m] \hbar^2 \langle \lambda m | \lambda m \rangle = |C_+|^2$$

or $[C_+|^2=(j-m)(j+m+1) \hbar^2$

$$\Rightarrow C_{+} = \sqrt{\{(j-m)(j+m+1)\}} \hat{n}$$
have chosen an arbit

where we have chosen an arbitrary phase factor as unity for

Thus we have

Thus we have
$$J_{+} \mid \lambda m \rangle = \sqrt{\{(j-m)(j+m+1)\}} \, \hbar \mid \lambda, m+1 \rangle \qquad ...(59a)$$
Similarly, we have

g these equations and the out
$$(59a)$$
 $(59a)$ $(59a)$

Using these equations and the orthonormality of the eigenkets $|\lambda m\rangle$ we can find out the explicit form of the matrices for the various generalized angular momentum operators for different

For j=0, J^2 and all components of J are represented by null matrix of order one.

For $j=\frac{1}{2}$, m will have the values $\frac{1}{2}$ and $-\frac{1}{2} \cdot \lambda$ will be equal to $j(j+1)=\frac{3}{4}$. Hence the matrix elements for J^2 and J_z are given by $\langle 3/4, m \mid J_z \mid 3/4, m' \rangle = m' \hbar \langle 3/4, m \mid 3/4, m' \rangle = m' \hbar \delta m m'.$

$$\langle 3/4, m \mid J^2 \mid 3/4, m' \rangle = m' \hbar \langle 3/4, m \mid 3/4, m' \rangle = m' \hbar \delta m m'.$$
The matrix elements of J_{-} and J_{-}

The matrix elements of J_+ and J_- can also be written in the common basis of J^2 and J_z :

$$\langle 3/4, m \mid J_{+} \mid 3/4, m' \rangle = \sqrt{\{(1/2 - m') (1/2 + m' + 1)\}}$$

$$= \sqrt{\{(1/2 - m') (1/2 + m' + 1)\} \, \ln \, \delta m, \, m' + 1}$$

$$J_z = \begin{bmatrix} m' & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{\hbar}{2} & 0 \\ -\frac{1}{2} & 0 & -\frac{\hbar}{2} \end{bmatrix}; \quad J^2 = \begin{bmatrix} m' & \frac{1}{2} & \frac{3\hbar^2}{4} & 0 \\ \frac{1}{2} & \frac{3\hbar^2}{4} & 0 \\ -\frac{1}{2} & 0 & \frac{3\hbar}{4} \end{bmatrix}$$

			<i>L.</i>		1 2		4
	m'	$\frac{1}{2}$	$-\frac{1}{2}$		m'	$\frac{1}{2}$	$-\frac{1}{2}$
$J_{+}=$	$\frac{1}{2}$	0	ħ		$\frac{1}{2}$	0	0
	$-\frac{1}{2}$	0	0	and $J_{-}=$	$-\frac{1}{2}$	'n	0

and $\langle 3/4, m \mid J_{-} \mid 3/4, m' \rangle = \sqrt{\{(1/2+m') (1/2-m'+1)\}}$ $\uparrow \land \langle 3/4, m \mid 3/4, m'-1 \rangle$ $= \sqrt{\{(1/2+m') (1/2-m'+1)\}} \uparrow \land \delta m, m'-1.$

Explicit form of the matrices are,

 $J_x = \frac{J_+ + J_-}{2} = \begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix}; J_y = \frac{J_+ - J_-}{2i} = \begin{pmatrix} 0 & -i\hbar/2 \\ i\hbar/2 & 0 \end{pmatrix}$

Similarly we find that, for j=1.

$$J_{x} = \frac{\hbar}{\sqrt{(2)}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \ J_{y} = \frac{\hbar}{\sqrt{(2)}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix};$$

$$J_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
 and $J^2 = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

and for j=3/2.

and

$$J_{x} = \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \end{pmatrix}; J_{y} = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\sqrt{3} & 0 & 0 \\ i\sqrt{3} & 0 & -2i & 0 \\ 0 & 2i & 0 -i\sqrt{3} \end{pmatrix}$$

$$J_{z} = \frac{\hbar}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \text{ and } J^{2} = \frac{15\hbar^{2}}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

7.9. ADDITION OF ANGULAR MOMENTA:

Let J_1 and J_2 be two independent (i.e. commuting) angular momentum vectors. J_1 may be the orbital angular momentum L and J_2 the spin S of some particle, or both may be the spin or orbital angular momenta of two different particles. Let us denote the sum of J_1 and J_2 by $J(J=J_1+J_2)$. Let J_2 , J_{12} and J_{22} be the z-components of J, J_1 and J_2 ; respectively. Since J_1 and J_2 commutes with each other while they separately satisfy the usual momentum J also satisfies the angular momentum commutation relations.

Now onwards we can designate the simultaneous eigenkets $\langle | \lambda m \rangle$ of J^2 and J_z by 'j' and 'm' as $\langle | j m \rangle$ ', because $\lambda = j$ (j+1). The eigenvalue equations (52) in these new notations can be written as:

$$J^{2} | j m \rangle = j (j+1) \hbar^{2} | j m \rangle \qquad ...(60a)$$

$$J_{z} | j m \rangle = m \hbar \quad j m \rangle \qquad ...(60b)$$

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Hence the orthonormal set of eigenkets of J_1^2 , J_{1z} can be written as $|j_1, m_1\rangle$ which forms the basis for a $(2j_1+1)$ dimensional vector space. Similarly, the eigenkets $|j_2, m_2\rangle$ of J_2^2 , J_{2z} are represented in a different vector space of dimension $(2j_2+1)$. The states of the coupled system are vectors in the direct product space of the two previously separated vector spaces.

Thus the problem of addition of two angular momenta consists of obtaining the eigen values of J^2 ; J_z and their eigenvectors in terms of the direct product of the eigenvectors of (J_1^2, J_{1z}) and (J_2^2, J_{2z}) . The normalized simultaneous eigenvectors of the four operators J_1^2 , J_2^2 , J_{1z} , J_{2z} can be symbolized by the direct product kets

$$|j_1m_1\rangle \otimes |j_2m_2\rangle \equiv |j_1j_2m_1m_2\rangle \qquad ...(61)$$

These constitute a basis for the product space. It is desired to construct from this basis the eigenvectors of (J^2, J_z) which forms a new basis. We write the eigenkets $|jm\rangle$ of J^2 and J_z as a linear combination of the eigenvectors (61) as

$$|jm\rangle = \sum_{m_1, m_2} C(j_1 j_2 m_1 m_2, jm) | j_1 j_2 m_1 m_2\rangle$$

Using the orthonormality of the eigenkets, the coefficients of expansion are given by

$$C\left(j_{1} j_{2} m_{1} m_{2}, j m\right) = \langle j_{1} j_{2} m_{1} m_{2} \mid j m\rangle.$$

$$\therefore |j m\rangle = \sum_{m_{1}, m_{2}} \langle j_{1} j_{2} m_{1} m_{2} \mid j m\rangle \mid j_{1} j_{2} m_{1} m_{2}\rangle. \qquad \dots (62)$$

Summation in (62) over m_1 is from $-j_1$ to j_1 and over m_2 from $-j_2$ to j_2 . The coefficients of expansion in (62) are known as the Clebsch-Gordan or wigner or Vector-coupling coefficients.

Now the question is: given the angular momenta (j_1, m_1) and (j_2, m_2) of the individual systems, what are the possible values of j and m for the composite system. For it we operate $J_z = J_{1z} + J_{2z}$ on (62)

$$J_{z} \mid jm \rangle = \sum_{m_{1}', m_{2}'} (J_{1z} + J_{2z}) \mid j_{1}j_{2}m_{1}'m_{2}' \rangle \langle j_{1}j_{2}m_{1}'m_{2}' \mid jm \rangle$$
or $m\hbar \mid jm \rangle = \sum_{m_{1}', m_{2}'} (m_{1}'\hbar + m_{2}'\hbar) \mid j_{1}j_{2}m_{1}'m_{2}' \rangle \langle j_{1}j_{2}m_{1}'m_{2}' \mid jm \rangle$
or $m \mid jm \rangle = \sum_{m_{1}', m_{2}'} (m_{1}' + m_{2}') \mid j_{1}j_{2}m_{1}'m_{2}' \rangle \langle j_{1}j_{2}m_{1}'m_{2}' \mid jm \rangle$

$$m_{1}', m_{2}'$$

or
$$m \langle j_1 j_2 m_1 m_2 | jm \rangle$$

$$= \sum_{m_{1}', m_{2}'} (m_{1}' + m_{2}') \langle j_{1} j_{2} m_{1} m_{2} | j_{1} j_{2} m_{1}' m_{2}' \rangle \langle j_{1} j_{2} m_{1}' m_{2}' | j_{m} \rangle$$

or $m \langle j_1 j_2 m_1 m_2 | jm \rangle$

$$= \sum_{m_{1}', m_{2}'} (m_{1}' + m_{2}') \, \delta_{m_{1}m_{1}} \, \delta_{m_{2}m_{2}'} \, \langle j_{1} j_{2} m_{1}' m_{2}' \mid jm \rangle$$

or
$$m \langle j_1 j_2 m_1 m_2 | jm \rangle = (m_1 + m_2) \langle j_1 j_2 m_1 m_2 | jm \rangle$$

or $m = m_1 + m_2$(63)

This is known as the triangle rule—2 for the addition of angular momenta and it states that the sum of the z-components of the angular momenta equals that of their resultant. Thus only those basis vectors will contribute for which this law is satisfied.

Next, we know that the largest value of m=j, and this occurs only once when m_1 and m_2 have their largest values, viz, j_1 and j_2 ; respectively. Thus from (63) we can say that the largest value of $j=j_1+j_2$ and there is only one such state for which this value is possible.

This second largest value of m is (j_1+j_2-1) and it can occur for two cases;

$${m_1=j_1 \atop m_2=j_2-1}$$
 and ${m_1=j_1-1 \atop m_2=j_2}$

There exist two linearly independent orthogonal combinations of these states which correspond to $j=j_1+j_2$ and j_1+j_2-1 and both with the projection (j_1+j_2-1) .

Next we choose $m=j_1+j_2-2$ which can be realized in three ways:

$$\left\{ \begin{array}{l}
 m_1 = j_1 \\
 m_2 = j_2 - 2
 \end{array} \right\}; \left\{ \begin{array}{l}
 m_1 = j_1 - 1 \\
 m_2 = j_2 - 1
 \end{array} \right\} \text{ and } \left\{ \begin{array}{l}
 m_1 = j_1 - 2 \\
 m_2 = j_2
 \end{array} \right\}.$$

It can be shown that there exist three orthogonal linear combinations of these states which correspond to $j=j_1+j_2$, j_1+j_2-1 and j_1+j_2-2 , all with projection equal to (j_1+j_2-2) .

Clearly, this sequence of arguments ends, if either m_1 or m_2 hits its lowest value, i.e., $m_1 = -j_1$ or $m_2 = -j_2$. The lowest value of j in that case will be $|j_1 - j_2|$. Thus j can have the values,

$$j_1+j_2 \leqslant j \leqslant |j_1-j_2|$$
. ...(64)

The is called the triangle rule—1 for the addition of angular momenta and it states that the magnitude of the sum of two angular momentum vectors can have any value ranging from the sum of their magnitude to the difference of their magnitude by integral steps.

7·10 RECURSION RELATION FOR CLEBSCH GORDAN (C. G.) COEFFICIENTS:

Simplifying the notations, we write $|j_1j_2m_1m_2\rangle \equiv |m_1m_2\rangle$, it is being understood that j_1 and j_2 are the maximum values of m_1 and m_2 . Hence we can write eqn. (62) as

$$|jm\rangle = \sum_{m_1, m_2} |m_1 m_2\rangle \langle m_1 m_2 | jm\rangle.$$

Applying the raising operator J_+ to the left hand side and the equal operator $(J_{1+}+J_{2+})$ to the right hand side of this equation, we get

tion, we get
$$J_{+} | jm \rangle = \sum_{m_{1}, m_{2}} \langle J_{1+} + J_{2+} \rangle | m_{1}m_{2} \rangle \langle m_{1}m_{2} | jm \rangle$$
or $\hbar \sqrt{\{(j-m)(j+m+1)\}} | j, m+1 \rangle$

$$= \sum_{m_{1}, m_{2}} [\hbar \sqrt{\{(j_{1}-m_{1})(j_{1}+m_{1}+1)\}} | m_{1}+1, m_{2} \rangle$$

$$+ \hbar \sqrt{\{(j_{2}-m_{2})(j_{2}+m_{2}+1)\}} | m_{1}, m_{2}+1 \rangle] \langle m_{1}m_{2} | jm \rangle$$
or $\langle m_{1}'m_{2}' | j, m+1 \rangle \sqrt{\{(j-m)(j+m+1)\}} \langle m_{1}'m_{2}' | m_{1}+1, m_{2} \rangle$

$$= \sum_{m_{1}, m_{2}} [\sqrt{\{(j_{1}-m_{1})(j_{1}+m_{1}+1)\}} \langle m_{1}'m_{2}' | m_{1}, m_{2}+1 \rangle]$$

$$+ \sqrt{\{(j_{2}-m_{2})(j_{2}+m_{2}+1)\}} \langle m_{1}, m_{2}' | m_{1}, m_{2}+1 \rangle]}$$

$$+ \sqrt{\{(j_{2}-m_{2}'+1)(j_{2}+m_{2}')\}} \langle m_{1}' | m_{2}' - 1 | jm \rangle ... (65a)}$$

$$\{ \because \langle m_{1}'m_{2}' | m_{1}+1, m_{2} \rangle = \delta_{m_{1}', m_{2}+1} \delta_{m_{2}', m_{2}}$$
and $\langle m_{1}'m_{2}' | m_{1}, m_{2}+1 \rangle = \delta_{m_{1}', m_{1}, m_{2}} \delta_{m_{2}+1} \}$,

Similarly, applying the lowering operator J_{-} , we get the

relation:

tion:

$$\langle m_1', m_2' | j, m-1 \rangle \sqrt{\{(j+m)(j-m+1)\}}$$

 $= \sqrt{\{(j_1+m_1'+1)(j_1-m_1')\}} \langle m_1'+1, m_2' | jm \rangle$
 $+ \sqrt{\{(j_2+m_2'+1)(j_2-m_2')\}} \langle m_1', m_2'+1 | jm \rangle$, ...(65 b)

Equations (65) are the desired recursion relations for the C. G. coefficients.

7.11. CONSTRUCTION OF C. G. COEFFICIENTS:

Now we describe the procedure for the construction of the C. G. coefficients, $\langle m_1 m_2 \mid jm \rangle$:

We know that for each values of j there are (2j+1) values of m associated with it. Also j can take values from $|j_1-j_2|$ to (j_1+j_2) . Hence the total number of $|jm\rangle$ states will be equal to

$$\sum_{j=|j_1-j_2|}^{j_1+j_2} (2j+1) = (2j_1+1) (2j_2+1).$$

Thus the matrix $\langle m_1 m_2 \mid jm \rangle$ has $(2j_1+1)$ $(2j_2+1)$ number of rows and the same number of columns, but breaks up into disconnected submatrices in accordance with the value of $m=m_1+m_2$.

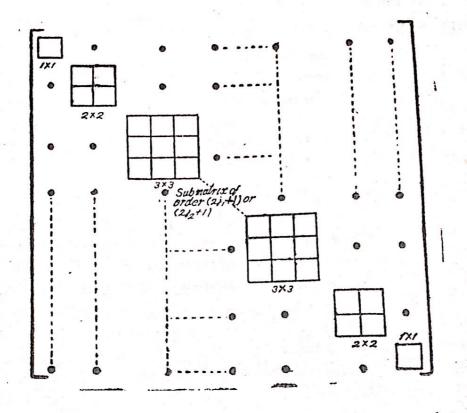
The highest values of $m=j=j_1-j_2$ and it occurs only once when $m_1=j_1$ and $m_2=j_2$. The next highest value of $m=j-1=j_1+j_2-1$ and it occurs twice when $m_1=j_1$, $m_2=j_2-1$ and $m_1=j_1-1$, $m_2=j_2$. Hence there will be a 1×1 submatrix, then a 2×2 submatrix and continuing like this we shall get a 3×3 submatrix, a 4×4 submatrix and so on until a maximum order is reached and maintained for one or more submatrices, then it decreases by unit steps till the last 1×1 submatrix has $m=-(j_1+j_2)$ and $j=(j_1+j_2)$. To find the maximum order of the submatrix we note that

for $m=j_1+j_2-0$, we get 1×1 submatrix, for $m=j_1+j_2-1$, we get 2×2 submatrix, for $m=j_1+j_2-2$, we get 3×3 submatrix, \vdots \vdots \vdots \vdots \vdots

for $m=j_1+j_2-n$, we get $(n+1)\times(n+1)$ submatrix.

Now $m=j_1+j_2-n$ can occur for $m_1=j_1$, $m_2=j_2-n$ and $m_1=j_1-n$, $m_2=j_2$. If $j_2-n\leqslant -j_2$, then $(n+1)\times (n+1)$ submatrix is not possible because the minimum value of m_2 can be $-j_2$. Similarly, $j_1-n\leqslant -j_1$ is also not possible. Thus the extreme value for it should be such that $j_2-n=-j_2$ or $j_1-n=-j_1$ i.e., $n=2j_2$ or $2j_1$ whichever is smaller. Hence the maximum order of the submatrix is (n+1)=(2j+1) or $(2j_2+1)$ whichever is smaller. So the general appearance of the C.G. coefficient matrix will be as shown in the table on page 248.

TABLE GENERAL FROM OF C G. COEFFICIENT MATRIX



As an explicit example the order of the various submatrices for $j_1=5/2$ and $j_2=1/2$ is shown in the table on page 249. The total dimension of the C.G. coefficient matrix is $(2j_1+1)(2j_2+1) = \left(2 \cdot \frac{5}{2} + 1\right) \left(2 \cdot \frac{1}{2} + 1\right) = 12$, and the maximum dimension of

the submatrix is
$$(2j_2+1)=(2\frac{1}{2}+1)=2$$
.

To evaluate the values of the elements of these submatrices, we shall make use of the following convensions:

- (i) All the elements $\langle m_1 m_2 | jm \rangle$ are real.
- (ii) We have $|jm\rangle = \sum_{m_1m_2} |m_1m_2\rangle\langle m_1m_2|jm\rangle$

$$\therefore \langle j'm' \mid j m \rangle = \delta j' j \ \delta m' m = \sum_{m_1 m_2} \langle j_1 j_2 m_1 m_2 \mid j m \rangle \times \langle j m' \mid j_1 j_2 m_1 m_2 \rangle$$

TABLE DIMENSIONS OF VARIOUS SUB-MATRICES FOR $j_1 = \frac{5}{2}$ AND $j_2 = \frac{1}{2}$.

					J. 6	-		<u> </u>				46.20
		j	3	3	2 3	2	3	2	3	2 3	2	3
	m_1	m	3	2	2 1	1	0	0	-1 -	-1 -2	-2	-3
1	<u>5</u>	1/2	(1×	1)	•		•		•	•	.	•
	$\begin{cases} \frac{5}{2} \\ 3 \\ 2 \end{cases}$	3 1 2	•	(2×	2) •		•		•			
	$\left\{\frac{3}{2}\right\}$	- 12 12 12	•		(2×	2)	•	ļ	•	•		•
-	$ \begin{cases} \frac{1}{2} \\ -\frac{1}{6} \end{cases} $	$-rac{1}{2}$	•	•	•	Ì	2×:	2)	•	•		•
•	$\begin{cases} -\frac{1}{2} \\ -\frac{3}{2} \end{cases}$	$-rac{1}{2}$	•		•	1	•		(2×2)	.		•
•	$ \begin{cases} -\frac{8}{2} \\ -\frac{5}{2} \end{cases} $	$-\frac{1}{2}\begin{vmatrix} 1\\1 \end{vmatrix}$	•		•		•		•	(2×	2)	•
_	$-\frac{5}{2}$	$-\frac{1}{2}$	•	•	•		•		•	•	(1	(×1)
	or	n	$\sum_{n_1m_2}$	$\langle j_1 j$	$m_1 m_1$	$_2 \mid jn$	$n > ^2$	=1			(66 a)

For the highest value of $j=j_1+j_2$ we have $m_1=j_1$ and $m_2=j_2$. then from eqn. (66) we have

$$|\langle j_1 j_2 j_1 j_2 | jj \rangle|^2 = 1 \Rightarrow \langle j_1 j_2 j_1 j_2 | jj \rangle = \pm 1.$$

We take here only +1 and discard the value -1.

Using the above two convensions, we shall find out the elements of the various submatrices. In order to find the elements of the 2×2 submatrix, we note that $m=j_1+j_2-1$ and j can have two values j_1+j_2 and j_1+j_2-1 . The various elements are tabulated below:

From the recurron relation (65b) with $m_1'=j_1$ and $m_2'=j_2-1$; $j=j_1+j_2$ and $m=j_1+j_2$ we get

$$\langle j_{1}, j_{2}-1 \mid j, j-1 \rangle = \frac{\sqrt{\{(j_{2}+j_{2}-1+1)(j_{2}-j_{2}+1)\}}\langle j_{1}j_{2} \mid jj \rangle}}{\sqrt{\{(j+j)(j-j+1)\}}}$$

$$= \sqrt{\left(\frac{2j_{2}}{2j}\right)} \quad \{ :: \langle j_{1}j_{2} \mid jj \rangle = 1 \}.$$

$$\therefore \langle j_{1}, j_{2}-1 \mid j, j-1 \rangle = \sqrt{\left(\frac{j_{2}}{j}\right)} = \sqrt{\left(\frac{j_{2}}{j_{1}+j_{2}}\right)} \qquad \dots (67-a)$$

To find the other elements of the first column we use the orthogonality relation (66-a). We write

or
$$|\langle j_{1}, j_{2} - 1 \mid j, j - 1 \rangle|^{2} + |\langle j_{1} - 1, j_{2} \mid j, j - 1 \rangle|^{2} = 1$$
or
$$\frac{j_{2}}{j_{1} + j_{2}} + |\langle j_{1} - 1, j_{2} \mid j, j - 1 \rangle|^{2} = 1$$

$$\Rightarrow \langle j_{1} - 1, j_{2} \mid j, j - 1 \rangle = \sqrt{\left(\frac{j_{1}}{j_{1} + j_{2}}\right)} \qquad \dots (67-b)$$

A relation analogus to (66-a) also holds for the elements of the various rows:

 $\sum_{jm} |\langle j_1 j_2 m_1 m_2 | jm \rangle|^2 = 1 \qquad ...(66-b)$

Using this relation for the rows of the above 2×2 submatrix, we get

$$\langle j_1, j_2 - 1 \mid j - 1, j - 1 \rangle = \sqrt{\left(\frac{j_1}{j_1 + j_2}\right)}$$
 ...(67-c)

and

$$\langle j_1 - 1, j_2 | j - 1, j - 1 \rangle = -\sqrt{\left(\frac{j_2}{j_1 + j_2}\right)}$$
 ...(67-d)

Various elements of the 3×3 submatrix are listed below.

1	j	j_1+j_2	$j_1 + j_2 - 1$	$j_1 + j_2 - 2$
		$j_1 + j_2 - 2$	j_1+j_2-2	j_1+j_2-2
j_1	$j_2 - 2$	$\langle j_1, j_2-2 \mid j$	$\langle j, j-2 \rangle, \langle j_1, j_2-2 \rangle$	$ j-1, j-2\rangle, j-1, j-2\rangle, j-2, j-2\rangle$
j_1-1	j_2-1	$\langle j_1-1, j_2-1 \rangle$	$ j,j-2\rangle, \langle j_1-1\rangle, \langle j_1-1\rangle$	$, j_2-1 \mid j-1, j-2\rangle, $ $1, j_2-1 \mid j-2, j-2\rangle$
				$ j-1, j-2\rangle$, $ j-2, j-2\rangle$

Putting $m_1'=j_1$; $m_2'=j_2-2$; $j=j_1+j_2$ and $m=j_1+j_2-1$ in eqn. (56-b) we get

$$\langle j_{1}, j_{2}-2 \mid j, j-2 \rangle, \sqrt{\{(2j-1).2\}}$$

$$= \sqrt{\{(2j_{2}-1).2\}} \langle j_{1} j_{2}-1 \mid j, j-1 \rangle$$
or $\langle j_{1}, j_{2}-2 \mid j, j-2 \rangle = \sqrt{\left(\frac{2j_{2}-1}{2(j_{1}+j_{2})-1}\right)} \cdot \langle j_{1}, j_{2}-1 \mid j, j-1 \rangle$

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Using eqn. (67-a), we get from it:

$$\langle j_1, j_2 - 2 \mid j, j - 2 \rangle = \left[\frac{j_2 (2j_2 + 1)}{(j_1 + j_2) (2j_1 + 2j_2 - 1)} \right]^{1/2}$$
 ... (68-a)

Again, putting $m_1'=j_1-1$, $m_2'=j_2-1$, $j=j_1+j_2$ and $m=j_1+j_2-1$ in eqn. (65-b) and using eqns. (67-a) and (67-b), we get

$$\langle j_1-1, j_2-1 \mid j, j-2 \rangle = \left[\frac{4j_1j_2}{(j_1+j_2)(2j_1+2j_2-1)} \right]^{1/2} \dots (68-b)$$

Now putting $m_1'=j_1-2$, $m_2'=j_2$, $j=j_1+j_2$ and $m=j_1+j_2-1$ in eqn. (65-b) and using eqn. (67-b), we get

$$\langle j_1-2, j_2 \mid j, j-2 \rangle = \left[\frac{j (2j_1-1)}{(j_1+j_2)(2j_1+j_2-1)} \right]^{1/2} \dots (68-c)$$

Similarly, using eqns. (65-b), (67-c) and (67-d), we can evaluate that

$$\langle j_1, j_2 \ 2 \ | \ j-1, j-2 \rangle = \left[\frac{j_1 \ (2j_2-1)}{(j_1+j_2)(j_1+j_2-1)} \right]^{1/2}, \quad \dots (68-d)$$

$$\langle j_1-1, j_2-1 | j-1, j-2 \rangle = \left[\frac{(j_1-j_2)^2}{(j_1+j_2)(j_1+j_2-1)} \right]^{1/2} \dots (68-e)^2$$

and

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$$\langle j_1-2, j_2 | j-1, j-2 \rangle = - \left[\frac{j_2 (2j_1-1)}{(j_1+j_2) (j_1+j_2-1)} \right]^{1/2} \dots (68-f)$$

We have constructed the elements of the first two columns of the 3×3 submatrix. In order to find out the elements of the third column, we use the orthogonality relation for the elements of a row. We obtain

$$\langle j_1, j_2 - 2 \mid j - 2, j - 2 \rangle = \left[\frac{j_1 (2j_1 - 1)}{(j_1 + j_2 - 1)(2j_1 + 2j_2 - 1)} \right]^{1/2}, \dots (68-g)$$

$$\langle j_1-1, j_2-1 \mid j-2, j-2 \rangle = -\left[\frac{(2j_1-1)(2j_2-1)}{(j_1+j_2-1)(2j_1+2j_2-1)} \right]^{1/2} \dots (68-h)$$

and

$$\langle j_1-2, j_2 | j-2, j-2 \rangle = \left[\frac{j_2 (2j_2-1)}{(j_1+j_2-1)(2j_1+2j_2-1)} \right]^{1/2} \dots (68-i)$$

As we go for the calculations of the elements of higher order submatrices, the process becomes very cumbersome. Hence the evaluation of the elements of a $n \times n$ submatrix is quite difficult and we don't try to evaluate them. Here we give some examples with particularly simple numerical values of j_1 and j_2 .

Example 1. If $j_1=j_2=\frac{1}{2}$, then the elements of the various submatrices are given by the following table:

		j m	-	1	0	1	36.7 S.		
m_1	m_2	1		0	0	-1 • •			
$\frac{1}{2}$	$-\frac{1}{2}$			//2	$1/\sqrt{2}$	 2		1,000	
$-\frac{1}{2}$	1/2		1	/1′2	$-1/\sqrt{2}$	•	}		
$-\frac{1}{2}$	$-\frac{1}{2}$		······································	•		······			

Example 2. For $j_1=1$ and $j_2=\frac{1}{2}$, the elements of the various submatrices are given by the following table:

In the above examples, the element of the first 1×1 submatrix is taken equal to unity by the convension. Elements of the next 2×2 submatrix are written by using equations (67).

To find out the elements of the next 2×2 submatrix we can apply the ladder down operation on the elements of the first 2×2 submatrix or we can also apply the ladder up operation on the elements of the last 1×1 submatrix. The recursion relation for the ladder up operation is given by equation (65-a). Putting $m_1 = -1$, $m_2 = +\frac{1}{2}$; $j = \frac{3}{2}$ and $m = -\frac{3}{2}$ in eqn. (65-a) and using the values of the elements of the first 2×2 submatrix, we have

$$\sqrt{3} \langle -1, \frac{1}{2} | \frac{3}{2}, -\frac{1}{2} \rangle = \langle -1, -\frac{1}{2} | \frac{3}{2}, -\frac{3}{2} \rangle = 1$$

$$\Rightarrow \langle -1, \frac{1}{2} | \frac{3}{2}, -\frac{1}{2} \rangle = \frac{1}{\sqrt{3}}.$$

Other elements can be obtained by using the orthogonality relations for the rows and the columns of a submatrix.

7.12. IDENTICAL PARTICLES WITH SPIN:

The partcles which can be substituted for each other without any change in the dynamical properties of the system constituted by them are known as "Identical particles". In classical mechanics, we can distinguish the identical particles of a system by following their paths of motion which are sharply defined trajectories. In quantum mechanics, due to the uncertainty principle, the position of a particle cannot be known definitely at a time even if we know it exactly at an infinitely close instant. The finite size and the spreading of the wavepackets for individual particles, make it impossible to distinguish between identical particles, especially when they interact with each other. Therefore, in quantum mechanics identical particles are indistinguishable, and hence all physically measurable quantities must be independent of the interchange of two particles.

Writing the Hamiltonian for a system of "n" identical particles by the symbol, H(1, 2, 3, ..., n) where 1, 2, 3 etc. denote the coordinates of first, second, third etc. particles; the principles of indistinguishability implies that the Hamiltonian is not affected by an interchange of the symbols that assign the coordinates to one or the other member of any pair of identical particles,

i.e.,
$$H(1, 2, 3, ..., n) = H(2, 1, 3, ..., n) = H(n, 1, 3, ..., 2)$$
 etc. ...(69)

In general, the Hamiltonian is unchanged by any permutation of the particle labels

Writing the wavefunction for "n" identical particles by the symbol, $\psi(1, 2, 3, ..., n)$, the Schroedinger equation for a system of "n" identical particles can be written as

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$$H(1, 2, 3, ..., n) \psi(1, 2, 3, ..., n) = i\hbar \frac{\partial \psi(1, 2, 3, ..., n)}{\partial t}$$
...(70)

If the symbols for the coordinates in eqn. (70) are permuted in any way, the resulting function ψ will also be a solution of equation (70), because the Hamiltonian remains unchanged by this permutation. In this way n! solutions can be obtained from a single one, each of which corresponds to one of the n! permutations of the n labels. These solutions are obviously degenerate with the original ψ . This is known as the excannge degeneracy.

Symmetric and antisymmetric Wavefunctions. A wavefunction $\psi(1, 2, 3, ..., n)$ is symmetric, if the interchange of any pair of particles among its arguments leaves the wavefunction unchanged. Wavefunction is antisymmetric.

We define the transposition operator $P_{ij}=P_{ji}$, which when operated on ψ , interchanges the *i*th and *j*th labels

 $P_{ij} \psi (1, 2, ..., i, ..., j, ..., n) = \psi (1, 2, ..., j, ..., i, ..., n)$. Thus any permutation of the particle labels can be obtained by the operations of the transposition operators.

Now, in quantum mechanics the wavefunction ψ (1, 2, 3, ,n) is to be interpreted as a probability amplitude for the system. The quantity $|\psi(1, 2, ..., n)|^2$ represents the probability density for the coordinates of the n particles. From the principle of indistinguishability of identical particles, the states ψ and $P\psi$ are in fact the same state, where P is the transposition operator for any permutation of the labels of the particles. Thus the quantities $|\psi(1, 2, ..., n)|^2$ and $|P\psi(1, 2, ..., n)|^2$ are the same. This means that the probability

 $|\psi(1, 2, ..., n)|^2 d^3r_1, d^3r_2, ..., d^3r_n$ is proportional to the probability that one of the particles is in the volume element $d^3r_1 d^3r_2 ... d^3r_n$, but nothing can be said as to which of the particles this may be. From the above discussion we can say that for every permutation P, ψ and $P\psi$ can differ only by a phase factor,

$$\psi(2, 1, 3, ..., n) = e^{i\alpha_{12}}\psi(1, 2, 3, ..., n),$$

where α_{12} is real and exp $(i\alpha_{12}) = \exp(i\alpha_{21})$ is the phase factor. By repeating the interchange, we get back the original wavefunction, while ψ is multiplied by $e^{i\alpha_{12}} \cdot e^{i\alpha_{21}} = e^{2i\alpha_{12}}$. It follows that

$$e^{2i\alpha_{12}}=1$$
, or $e^{i\alpha_{12}}=\pm 1$. Thus $\psi(2, 1, 3, ..., n)=\pm \psi(1, 2, 3, ..., n)$

and the same is true for the interchange of any pair of particles. In the above, the wavefunction is symmetrical when interchange of particles leaves it unchanged and antisymmetrical when this interchange changes the sign. Therefore, the wavefunction which describes a physical state of a system containing any number of identical particles must be either symmetric or antisymmetric with respect to permutations of the labels of the particles. Of the n! solutions of eqn. (70) obtained by permuting the particle labels,

only two linear combinations can describe physical states; A symmetric solution can be obtained by taking the sum of all these n! solutions because the interchange of any pair of particles changes any one of the component functions into another of them and the latter into the former, leaving the entire wavefunction unchanged. An antisymmetric wavefunction can be constructed by adding together all the permuted functions that arise from the original function by means of an even number of interchanges of pairs of particles, and subtracting the sum of all the permuted functions that arise by means of an odd number of interchanges of pairs of particles in the original solution.

It should be noted that the symmetry character of a wavefunction is permanent, and a system which is at one instant in a symmetric (or antisymmetric) state remains so far all times, show it let ψ be symmetric at a particular time t. Then $H\psi$ is also symmetric because H does not change by any permutation of labels. Hence from eqn. (70) $\partial \psi / \partial t$ is also symmetric. Since ψ and its time derivative are symmetric at time t, ψ at an infinitesimally later time (t+dt) is given by $\left(\psi + \frac{\partial \psi}{\partial t} dt\right)$ and symmetric. Such a step by step integration of the wave equation can be continued for arbitrary large time intervals, and ψ is seen to remain symmetric always. Similarly, if ψ is antisymmetric at any time t, $H\psi$ and hence $\partial\psi/\partial t$ are antisymmetric, and integration of the wave equation shows that ϕ is always antisymmetric. Thus any sort of interaction is unable to make a transition between syinmetric and antisymmetric states. Only one of the two symmetry types ever occurs for a given type of particles, and the linear combinations of the two symmetry types do not occur.

Pauli's exclusion principle. By comparing theoretical predictions with experimental observations, it has been found that systems of particles with half integral spin (electrons, protons, neutrons etc.) from totally antisymmetrical states only, and the systems of particles with zero or integral spin (photons, π -mesons etc.) form totally symmetrical states only. Particles described by symmetrical wave functions are said to obey Bese-Einstein statistics and are called bosons. The particles which are described by antisymmetrical wavefunctions are said to obey Fermi-Dirac statistics and are called fermions. Thus the wavefunction for a system of fermions should be antisymmetrical and that for

a system of bosons should be symmetrical. We have described that how to construct the symmetrical and antisymmetrical wavefunctions for a system of "n" identical particles. If there is no interaction between the particles, then the Hamiltonian can be written as the sum of equal Hamiltonian functions for the separate particles:

H(1, 2, 3, ..., n) = H(1) + H(2) + H(3) + ... + H(n) ...(71) and the wavefunction will be a product of one particle eigenfunctions of H(1), H(2), etc., i.e.

 $\psi(1, 2, 3, ..., n) = \psi_1(1) \psi_2(2) \psi_3(3) ... \psi_n(n), ...(72)$

where

$$H(i) \psi_i(i) = E_i \psi_i(i) ; i=1, 2, 3, ..., n.$$

The subscripts of the single particle functions in (72) tell us the position of the particles while the arguments of the functions specify all of their coordinates and spin. We can make n! functions of the form (72) by permutation of the particle labels. The antisymmetric combination of these n! functions can be formed

$$\psi_{A}(1, 2, ..., n) = \frac{1}{\sqrt{(n !)}} \sum_{P} (-1)^{P} P \psi_{1}(1) \psi_{2}(2) \psi_{3}(3) ... \psi_{n}(n);$$
the symbol Σ denotes the sum over $n !$ functions obtained by

permuting the particle labels, and $(-1)^p$ is +1 or -1, depending on whether the permutation P can be represented as an even or an odd number of transpositions. $\frac{1}{\sqrt{(n!)}}$ is the normalization constant of the wavefunction. We can express (73) as a determinant known as the Slater's determinant:

$$\psi_{A}(1, 2, ..., n) = \frac{1}{\sqrt{(n \, !)}} \begin{bmatrix} \psi_{1}(1) & \psi_{1}(2) & ... & \psi_{1}(n) \\ \psi_{2}(1) & \psi_{2}(2) & ... & \psi_{2}(n) \\ ... & ... & ... \\ \psi_{n}(1) & \psi_{n}(2) & ... & \psi_{n}(n) \end{bmatrix} ... (74)$$

The symmetric combination is given by

$$\psi_{S}(1, 2, ..., n) = \frac{1}{\sqrt{(n !)}} \sum_{P} P \psi_{1}(1) \psi_{2}(2)... \psi_{n}(n) ...(75)$$

From eqn. (74) we see that the interchange of two particles is equivalent to an interchange of two rows of the determinant which therefore changes its sign. Also, if we put two particles in

the same position, then the rows of the determinant correspond. ing to these positions become identical and hence the determinant vanishes. Thus no two (or more) fermions can exist in the same state at the same time. This is called the Pauli's exclusion principle. However, eqn. (75) is never zero; there is no exclusion principle for bosons.

As an example, if two electrons in an atom have the same values of the quantum numbers n, l and m; the directions of their spins must be antiparallel. The probability of finding the two electrons with the same spin simultaneously at the same point is zero. Clearly the number of fermions in any state is 0 or 1. On the other hand, there is no such restriction on the number of bosons in any state.

7-13. ROTATIONS AND ANGULAR MOMENTA:

Let a quantum mechanical state $|\psi\rangle$ goes over into a state $|\psi'\rangle$ as a result of a rotation through some angle about some axis. Fig. I shows a rotation through an angle θ about the z-axis. Let this operation be carried out by an operator U. Then

 $U \mid \psi \rangle = \mid \psi' \rangle$.

When we say that the state $|\psi\rangle$ goes over into the state $|\psi'\rangle$ after

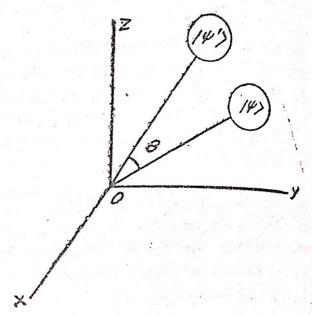


Fig. 1. Rotation about z-axis through an angle v.

the rotation, we mean that whatever observations we make upon the system in state $|\psi'\rangle$, the results of these observations can be deduced by rotation from the results that the same observation would yield if made upon the system in state $|\psi\rangle$.

We require that $|\psi\rangle$ should be normalized for normalized $|\psi\rangle$; hence

$$\langle \psi' \mid \psi' \rangle = \langle \psi \mid \psi \rangle$$
or
$$\langle \psi' \mid U \dagger U \mid \psi \rangle = \langle \psi \mid \psi \rangle$$

$$\Rightarrow U \dagger U = 1 \; ; i.e. \; U \text{ is unitary.} \qquad ...(76)$$

Thus the rotation of the states is represented by a unitary

operator *U* which should depend only on the relative orientations of the system, before and after the rotation.

Having defined the transformation of state vectors under rotation, we now define the transformation of observables. Let A be an observable which transforms into A' after the rotation U. Physically, the transformation of A into A' represents an overall rotation of the measuring instrument. Therefore, the average value of measurements of A made in the state $|\psi\rangle$ is equal to the average value of measurements of A' made in the state $|\psi\rangle$; i.e.,

$$\langle \psi \mid A \mid \psi \rangle = \langle \psi' \mid A' \mid \psi' \rangle = \langle \psi \mid U \dagger A' U \mid \psi \rangle$$
i.e.
$$A' = UAU \dagger \qquad ...(77)$$

Thus, in a rotation, the observables undergo the same unitary transformation as the state vectors.

Now we establish the fundamental relation between the angular momentum of a system and its infinitesimal rotation operators:

Let a rotation by an infinitesimal angle " ϵ " about z-axis, transforms $(x, y, z) \rightarrow (x', y', z')$ then

$$x' = x \cos \epsilon - y \sin \epsilon \approx x - y \epsilon y' = x \sin \epsilon + y \cos \epsilon \approx x \epsilon + y z' = z$$
 ...(78)

{: for very-very small ϵ , $\sin \epsilon \approx \epsilon$ and $\cos \epsilon \approx 1$ }

or
$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}; \qquad \dots (79)$$

ie., a small rotation " ϵ " about z-axis corresponds to a matrix very near to the unit matrix. Hence a rotation about any axis in the direction of the unit vector \hat{n} can be represented by the unitary matrix

$$U = \left(I - \frac{i\epsilon}{\hbar} \hat{n} \cdot J\right); \qquad ...(80)$$

where J represents the generator of rotation and \hat{n} . J is its component in the direction of vector \hat{n} . The factor $\frac{i}{\hbar}$ has been introduced for later convenience. From the unitarity of U, we have,

$$I = U \dagger U = \left[I + \frac{i\epsilon}{\hbar} (\hat{n} \cdot \mathbf{J}) \dagger \right] \left[I - \frac{i\epsilon}{\hbar} (\hat{n} \cdot \mathbf{J}) \right]$$

1

$$I = I + \frac{i\epsilon}{\hbar} (\hat{n}.\mathbf{J}) \dagger - \frac{i\epsilon}{\hbar} (\hat{n}.\mathbf{J}) ;$$

neglecting square and higher power terms in ϵ .

Thus we have

we have
$$\frac{i\epsilon}{\hbar} (\hat{n} \mathbf{J}) \dagger - \frac{i\epsilon}{\hbar} (\hat{n} \cdot \mathbf{J}) = 0 \Rightarrow (\hat{n} \cdot \mathbf{J}) \dagger = (\hat{n} \cdot \mathbf{J});$$

ie... the component of J in the direction of an arbitrary unit vector \hat{n} is Hermitian and hence J itself is also Hermitian. We also show that J is a vector operator. For it we have

$$|\psi'\rangle = \left(1 - \frac{i\epsilon}{\hbar} \hat{n} \cdot \mathbf{J}\right) |\psi\rangle$$

$$\therefore \langle \psi | \psi'\rangle = \langle \psi | \psi \rangle - \frac{i\epsilon}{\hbar} \hat{n} \cdot \langle \mathbf{J} \rangle$$

where $\langle J \rangle$ is the expectation value of J in the state $|\psi\rangle$. If we now apply an arbitrary finite rotation simultaneously to the states $|\psi\rangle$ and $|\psi'\rangle$, the scalars $\langle\psi|\psi'\rangle$ and $\langle\psi|\psi\rangle$ will be invariant. Hence the scalar product \hat{n} . $\langle J \rangle$ will also be rotationally invariant; i.e. it should be a scalar. As \hat{n} is a vector, $\langle J \rangle$ should also be a vector, and thus J is a vector operator. We shall denote by J_x , J_y and J_z ; the components of it along the x, y and z-axis; respectively.

In order to identify J, let us consider an arbitray vector operator A. Then

$$\begin{bmatrix}
\langle \psi' \mid A_x \mid \psi' \rangle \\
\langle \psi' \mid A_y \mid \psi' \rangle \\
\langle \psi' \mid A_z \mid \psi' \rangle
\end{bmatrix} = R_{3\times3} \begin{bmatrix}
\langle \psi \mid A_x \mid \psi \rangle \\
\langle \psi \mid A_y \mid \psi \rangle \\
\langle \psi \mid A_z \mid \psi \rangle
\end{bmatrix}$$

where $R_{3\times3}$ is a matrix of order 3 which gives the transformation from the values of the components of A in the state $|\psi\rangle$ to that in the state $|\psi'\rangle$. Since $|\psi'\rangle = U|\psi\rangle$, we can write from above as

$$\begin{array}{c}
U \dagger A_{x} U = R_{11} A_{x} + R_{12} A_{y} + R_{13} A_{z} \\
U \dagger A_{y} U = R_{21} A_{x} + R_{22} A_{y} + R_{23} A_{z} \\
U \dagger A_{z} U = R_{31} A_{x} + R_{32} A_{y} + R_{33} A_{z}
\end{array}$$
...(81)

If we take the vector operator A, in a particular case, as the position operator r with components x, y and z; we see from eqn. (79) that for a rotation about z-axis through an infinitesimal angle ϵ ,

$$R_{3\times 3} = \begin{bmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
 ...(82)

Hence for a rotation through an infinitesimal angle ":e" about z-axis, we can write from the first of eqns. (81) as,

$$\left(I + \frac{i\epsilon}{\hbar} J_z\right) A_x \left(I - \frac{i\epsilon}{\hbar} J_z\right) = A_x - \epsilon A_y + 0 A_z$$

$$\left\{ \because U - \left(I - \frac{i\epsilon}{\hbar} J_z\right) \text{ for a rotation about } z\text{-axis} \right\}$$

$$\frac{[i\epsilon]}{\hbar} J_z A_x - \frac{i\epsilon}{\hbar} A_x J_z = -\epsilon A_y$$

or

From the other two eqns. (81); $J_z A_y - A_y J_z = -i \hbar A_x$ $J_z A_z - A_z J_z = 0$ $J_z A_z - A_z J_z = 0$

and

Similarly, rotations about the x-and y-axes give the relations:

$$\begin{cases}
J_x A_y - A_y J_x = i\hbar A_z \\
J_x A_z - A_z J_x = -i\hbar A_y \\
J_x A_x - A_x J_x = 0
\end{cases}$$
...(83b)

and

$$\begin{cases}
 J_y A_z - A_z J_y = i \hbar A_z \\
 J_y A_x - A_x J_y = -i \hbar A_z \\
 J_y A_y - A_y J_y = 0
 \end{cases}
 ...(83c)$$

We have not put any restriction on the vector operator A. It can be any general vector operator, and in particular, if we take $A \equiv J$, then from equations (83) we see that,

$$\begin{cases}
J_{x} J_{y} - J_{y} J_{x} = i \ln J_{z} \\
J_{y} J_{z} - J_{z} J_{y} = i \ln J_{x} \\
J_{z} J_{x} - J_{x} J_{z} = i \ln J_{y}
\end{cases}$$
...(84)

i.e., the components of J satisfy the commutation relations of the angular momentum operator. Hence the generator "J" of an infinitesimal ratation is identical with the orbital angular momentum of the system.

Now, a finite rotation θ about the axis \hat{n} can be constructed by an infinite sequence of infinitesimal rotations ' ϵ ' about \hat{n} . Therefore the matrix for a finite rotation θ , can be written from eqn. (80) as

$$U^{(J)}(\theta) = \lim_{n \to \infty} \left(1 - \frac{i}{\hbar} \cdot \frac{\theta}{n} \hat{n} \cdot J \right)^{n}$$

$$= \exp \left\{ -\frac{i}{\hbar} \hat{n} \cdot J \theta \right\} \qquad \dots (85)$$

Hence, for a rotation θ about \hat{n} we have :

$$|\psi'\rangle = \exp\left\{-\frac{i}{\hbar}\hat{n}.\mathbf{J}\,\theta\right\}|\psi\rangle \qquad ...(86)$$

and

$$A' = \exp \left\{-\frac{i}{\hbar}\hat{n}.J \theta\right\} A \exp \left\{\frac{i}{\hbar}\hat{n}.J \theta\right\} \dots (87)$$

7.14. IRREDUCIBLE TENSOR OPERATORS:

In order to define an irreducible tensor operator, we begin with the definition of an irreducible linear vector space: Let V_x be an n-dimensional linear vector space spanned by the basis vectors $|u_1\rangle, |u_2\rangle, \ldots, |u_n\rangle$. If a transformation changes these basis vectors into the new vectors $|u_1\rangle, |u_2\rangle, \ldots, |u_n\rangle$ and if these new vectors also span the same space V_n then the vector space V_n is known as irreducible with respect to the given transformation. Now it is well known that the fundamental characteization of a tensor is through the linear transformations of its components under the effect of a specified class of operations (such as rotations) on the coordinate system. Thus the vectors of V_n are n-component tensors. By definition, a tensor is irreducible, if the space V_n in which it is defined is irreducible.

We have seen in the previous section that if $|\psi\rangle$ is any state vector, and A an operator representing some dynamical variable,

the rotation through an infinitesimal angle ' ϵ ' about the direction \hat{n} takes $|\psi\rangle$ and A into $|\psi'\rangle$ and A', where

 $|\psi'\rangle \approx \left(I - \frac{i\epsilon \hat{n}}{\hbar} \hat{n}.J\right) |\psi\rangle$ $A' \approx \left(I - \frac{i\epsilon \hat{n}}{\hbar} \hat{n}.J\right) A\left(I + \frac{i\epsilon \hat{n}}{\hbar} \hat{n}.J\right)$ $\approx A - \frac{i\epsilon \hat{n}}{\hbar} \hat{n}.[J,A]$

and

Thus the changes in $|\psi\rangle$ and A, brought about by infinite-simal rotations, are directly expressed in terms of $J |\psi\rangle$ and [J, A]; respectively. In our discussion, we shall find it to be convenient to work with the *spherical components* (also known as the *standard components*) of the vector J rather then the cartesian components. These are defined by

$$J_1 = -(J_x + i J_y)/\sqrt{(2)} = -1/\sqrt{(2)} J_+, J_0 = J_z$$

and $J_{-1} = (J_x - i J_y)/\sqrt{(2)} = 1/\sqrt{(2)} J_-$...(88)

The commutation relations of these operators can be written from eqns. (51). It can very eassily be verified that

$$[\mathbf{J}_{\mu}, \mathbf{J}_{\nu}] = \sum_{\mu'} \mathbf{J}_{\mu'} \langle 1\mu' \mid \mathbf{J}_{\mu} \mid 1 \nu \rangle \qquad ...(89)$$

Using the fact that

$$\langle 1\mu' \mid \mathbf{J}_0 \mid 1\mu \rangle = \langle 1\mu' \mid J_z \mid 1\mu \rangle = \mu \hbar \delta_{\mu\mu'}$$

$$\langle 1\mu' \mid \mathbf{J}_{\pm 1} \mid 1\mu \rangle = \mp \frac{1}{\sqrt{(2)}} \langle 1 \mu' \mid J_{\pm} \mid 1\mu \rangle$$

$$= \mp [1 - \frac{1}{2} (\mu^2 \pm \mu)]^{1/2} \hbar \delta_{\mu'}, \ \mu \pm 1.$$

New we observe that if $|\psi\rangle$ is any of the angular momentum states $|jm\rangle$, then the change $J_{\mu}|\psi\rangle = J_{\mu}|jm\rangle$ is all inear combination of states having the same j and various m. Specifically,

$$\mathbf{J}_{\mu} \mid jm\rangle = \frac{\Sigma}{m'} \mid jm'\rangle \langle jm' \mid \mathbf{J}_{\mu} \mid jm\rangle \qquad ...(90)$$

Thus the (2j+1) states $|jm\rangle$ transform linearly among themselves when subjected to a rotation and therefore, for a given j form an irreducible tensor of rank j, with (2j+1) components labelled by m=j, j-1, ..., -j. The transformation operation is the rotation about the origin.

We consider now the changes $[J_{\mu}, A]$ in operators A: Suppose we have a set of (2j+1) operators (which we shall denote by $T_{m}^{(j)}$, m=j, j-1, ..., -j) such that under commutation with the J_{μ} , the set undergoes the same linear transformation as the state $|jm\rangle$; i.e.,

$$\begin{bmatrix} \mathbf{J}_{\mu}, T_{m}^{(j)} \end{bmatrix} = \sum_{m'} T_{m'}^{(j)} \langle jm' \mid \mathbf{J}_{\mu} \mid jm \rangle. \qquad ...(91)$$

Then the set of operators $T_m^{(j)}$ constitute an irreducible tensor operator of rank j with (2j+1) components corresponding to (2j+1) values of m. Eqn. (91) provides an alternative definition of an irreducible tensor operator. This definition is due to Racah and it states that the (2j+1) operators $T_m^{(j)}$ are said to be the standard components of an irreducible tensor operator $T^{(j)}$ if they satisfy the above commutation relation with the components of the angular momentum operatur J. Eqn. (91) can be written equivalently as:

$$\begin{bmatrix} J_z & T_m^{(j)} \\ J_{\pm}, & T_m^{(j)} = \end{bmatrix} j (j+1) - m (m\pm 1). \end{bmatrix}^{1/2} \hbar T_{m\pm 1}^{(j)}$$
...(92)

7.15. THE WIGNER-ECKART THEOREM:

The matrix elements of the tensor operators between the eigenstates are of great physical importance. The Wigner-Eckart theorem gives the ratio of the matrix elements of a tensor operator between angular momentum eigenstates in terms of C. G. coefficients. This greatly simplifies the calculations because all the matrix elements of a tensor operator can be related to one particular element which may be chosen to be the simplest one and is usually determined experimentally.

One putting in the other quantum numbers explicitly, the Wigner-Eckart theorem gives the matrix element $\langle N_1 j_1 m_1 | T_m^{(j)}$ $| N_2 j_2 m_2 \rangle$ of any component of a tensor operator as:

$$\langle N_1 j_1 m_1 | T_m^{(j)} | N_2 j_2 m_2 \rangle = \langle N_1 j_1 || T^{(j)} || N_2 j_2 \rangle$$

 $\langle j_2 j m_2 m | j_1 m_1 \rangle ... (93)$

The parameters N_1 and N_2 appearing here stands for one or more quantum numbers required for a complete specification of basis states when such extra degress of freedom are present, - e.g., the principal quantum number will be such a degree of freedom in the case of hydrogen atom.

In eqn. (93), $\langle N_1 j, || T^{(j)} || N_2 j_2 \rangle$ depends only on the nature of the tensor operator and the quantum numbers N_1 , j_1 , N_2 and j_2 . It is independent of m, m_1 and m_2 . It is known as the reduced matrix element or the double-bar matrix element. (It is not a matrix element in the quantum mechanical sense, hence the use of double bars is make). $\langle j_2 j m_2 m | j_1 m_1 \rangle$ is the C.G. coefficient which is quite independent of the physical nature of the tensor operator. Expressed in words, eqn. (93) states that the matrix element of the m-th standard component of a tensor operator $T^{(j)}$ between the angular momentum eigenstates $|N_1 j_1 m_1 \rangle$ and $|N_2 j_2 m_2 \rangle$ equals the product of the C.G. coefficient $\langle j_2 j m_2 m | j_1 m_1 \rangle$ with a number which is independent of m, m_1 and m_2 .

Proof. The proof of the theorem follows almost trivially from the basic definition of tensor operators. On taking the matrix element of Eq. (91) we obtain

$$\sum_{m'} \langle N_1 j_1 m_1 \mid T_{m'}^{(j)} \mid N_2 j_2 m_2 \rangle \langle jm' \mid \mathbf{J}_{\mu} \mid jm \rangle$$

$$= \langle N_{1} j_{1} m_{1} | \left[J_{\mu}, T_{m}^{(j)} \right] | N_{2} j_{2} m_{2} \rangle$$

$$= \sum_{m''} \left\{ \langle j_{1} m_{1} | J_{\mu} | j_{1} m'' \rangle \langle N_{1} j_{1} m'' | T_{m}^{(j)} | N_{2} j_{2} m_{2} \rangle$$

$$- \langle N_{1} j_{1} m_{1} | T_{m}^{(j)} | N_{2} j_{2} m'' \rangle \langle j_{2} m'' | J_{\mu} | j_{2} m_{2} \rangle \right\} ...(94)$$

Here we have introduced the projection operator

$$1 = \sum_{N''j''m''} |N''j''m''\rangle \langle N''j''m''|$$

between J_{μ} and $T_{m}^{(j)}$, and used the fact that

$$\langle N_1 j_1 m_1 | J_{\mu} | N'' j'' m'' \rangle = \langle j_1 m_1 | J_{\mu} | j_2 m_2 \rangle \delta N_1 N'' \delta j_1 j''.$$

On the other hand we can obtain an equation of identical form with C.C. coefficients in place of the matrix elements. Specifically,

$$\sum_{m'} \langle j_1 m_1 \mid j_2 j m_2 m' \rangle \langle j m' \mid \mathbf{J}_{\mu} \mid j m \rangle$$

$$= \sum_{m''} \{ \langle j_1 m_1 \mid \mathbf{J}_{\mu} \mid j_1 m'' \rangle \langle j_1 m'' \mid j_2 j m_2 m \rangle$$

$$-\langle j_1 m_1 | j_2 j m'' m \rangle \langle j_2 m'' | \mathbf{J}_{\mu} | j_2 m_2 \rangle \} \qquad \dots (95)$$

This equation follows from the identity

$$\langle j_1 m_1 \mid J_{\mu} \mid j_2 j m_2 m \rangle \equiv \sum_{m''} \langle j_1 m_1 \mid J_{\mu} \mid j_1 m' \rangle$$

$$\times \langle j_1 m'' \mid j_2 j m_2 m \rangle \dots (96)$$

on re-expressing the left hand side as

and writing $J_{\mu} = J_{1\mu} + J_{2\mu}$, where $J_{1\mu}$ acts on the $j_2 m_2$ variables only and $j_{2\mu}$ on the jm, the last factor in the above eqn. can be written as

$$\langle j_2 m'' | \mathbf{J}_{1\mu} | j_2 m_2 \rangle \delta m'' m + \langle jm' | \mathbf{J}_{2\mu} | jm \rangle \delta m'' m_2$$

Hence the above eqn., or what is the same thing, the left hand side of eqn. (96), becomes

$$\sum_{m''} \langle j_1 m_1 \mid j_2 j m'' m \rangle \langle j_2 m'' \mid \mathbf{J}_{\mu} \mid j_2 m_2 \rangle$$

$$+\sum_{m'}\langle j, m_1 \mid j_2 j m_2 m' \rangle \langle j m' \mid \mathbf{J}_{\mu} \mid j m \rangle \qquad ... (97)$$

with this, eqn. (96) reduces to Eqn. (95)†.

Now, let us compare Eq. (94), ignoring the middle member, with Eq. (95). The two are identical except that $\langle N_1 j_1 m_1 | T^{(j)} m' | N_2 j_2 m_2 \rangle$ in one is replaced by $\langle j_1 m_1 | j_2 m_2 m' \rangle$ in the other. Evidently the two equations can be mutually consistent if and only if the above two quantities are proportional to each other, with a proportionality factor independent of the summation indices occurring in the equations (i.e. the magnetic quantum numbers). This is precisely what is stated by the Wigner-Eckart theorem, eqn. (93). This completes the proof.

The matrix elements (93) has the same selection rules as the C.G. co-efficients appearing in it; i.e., they vanishes unless $|j-j_2| \le j_1 \le j+j_2$, $m_1=m+m_2$ and $|m_1| \le j_1$. Once the reduced matrix element $\langle N_1 j_1 || T^{(j)} || N_2 j_2 \rangle$ is determined for given values of j_1 , $-j_2$, N_1 and N_2 , all the $(2j_2+1)$ (2j+1) (2j+1) matrix elements can be easily obtained from tables of C.G. coefficients. Moreover, taking the ratio of any two matrix elements of the same tensor operator of the form (93), we find that

$$\frac{\langle N_{1} j_{1} m_{1} | T_{m}^{(i)} | N_{2} j_{2} m_{2} \rangle}{\langle N_{1} j_{1} m' | T_{m'}^{(j)} | N_{2} j_{2} m'_{2} \rangle} = \frac{\langle j_{2} j m_{2} m | j_{1} m_{1} \rangle}{\langle j_{2} j m_{2}' m' | j_{1} m' \rangle}$$

Thus the ratios of the matrix elements are determined without any other knowledge.

It is not an easy task to calculate the reduced matrix element theoretically. It is normally determined from wigner-Eckart Theorem by calculating one particular element experimentally. This is usually chosen to be the one simplest to observe, that for which $m_1=m_2=0$ or 1 and m=0 dependend on whether the system has integral or half integral angular momentum. The Wigner-Eckart theorem has useful applications in atomic and nuclear physics.

[†]We drop the subscripts 1 and 2 on $j_{1\mu}$ and $j_{2\mu}$, with the understanding that J_{μ} stands for angular momentum operator which pertains to the system concerned.

Example. The Quadrupole Moment. The quadrupole moment of charge distribution $\rho(\mathbf{r})$ which has axial symmetry is defined

$$Q = \int (3z^2 - r^2) \rho (\mathbf{r}) d^3r,$$

where axis of symmetry is the z-axis and the origin is chosen as the centre of charge.

In quantum mechanics, a particle of charge e with the wavefunction ψ (r), produces a charge distribution ρ (r)=e ψ * (r) ψ (r)

$$Q = e \int \psi^* (\mathbf{r}) (3z^2 - r^2) \psi (\mathbf{r}) d^3r$$

Now, $(3z^2-r^2)$ is the component $Q_0^{(2)}$ of a second rank tensor operator. Observe that in the terms of spherical harmonics Y_l^m , $Q_0^{(2)} \equiv (3z^2-r^2) = \sqrt{\left(\frac{16\pi}{5}\right)r^2} Y_2^0$. Therefore, if ψ is the angular momentum state $|lm\rangle$, we have from the Wigner-Eckart theorem that

$$\langle lm \mid Q_0^{(2)} \mid lm \rangle = \langle l \parallel Q^{(2)} \parallel l \rangle \langle l \mid 2m \mid 0 \mid lm \rangle$$

It is the value of this quantity when m=l which is usually referred to as the quadrupole moment Q in a quantum state of angular momentum l. With this definition,

$$\langle l m \mid Q_0^{(2)} \mid l m \rangle = Q \frac{\langle l \mid 2m \mid 0 \mid l \mid m \rangle}{\langle l \mid 2 \mid l \mid 0 \mid l \mid l \rangle} = Q \frac{3m^2 - l \cdot (l+1)}{l \cdot (2l-1)}.$$
PROBLEMS

Problem 1. Show that for a particle moving in a conservative potential $V(\mathbf{r})$,

$$[H, L_z] = i\hbar \frac{\partial V(\mathbf{r})}{\partial \phi} and [H, L^2] = [V, L^2],$$

and hence prove that the orbital angular momentum is a constant of motion for the central field problem.

Sol. The Hamiltonian for a particle moving in a conservative field can be written as

$$H = \frac{p^2}{2m} + V(\mathbf{r}). \qquad \dots (i)$$

$$\therefore [H, L_z] = \left[\frac{p^2}{2m} + V(\mathbf{r}), L_z\right] = \frac{1}{2m} [p^2, L_z] + [V(\mathbf{r}), L_z]$$

...(ii)

Now,
$$[p^2, L_z] = [p_x^2 + p_y^2 + p_z^2, L_z]$$

 $= [p_x^2, L_z] + [p_y^2, L_z] \quad \{ \because P_z \text{ commutes with } L_z \}$
 $= p_x [p_x, L_z] + [p_x, L_z] p_x + p_y [p_y, L_z,]$
 $+ [p_y, L_z] p_y$
 $= -i \ln p_x p_y - i \ln p_y p_x + i \ln p_y p_x + i \ln p_x p_y = 0$
and $[V(\mathbf{r}), L_z] = \begin{bmatrix} V(\mathbf{r}), -i \ln \frac{\partial}{\partial \phi} \end{bmatrix}$
 $= -i \ln V(\mathbf{r}) \frac{\partial}{\partial \phi} + i \ln V \frac{\partial}{\partial \phi} + i \ln \frac{\partial V(\mathbf{r})}{\partial \phi}$
 $= i \ln \frac{\partial V(\mathbf{r})}{\partial \phi}$
Hence, $[H, L_z] = i \ln \frac{\partial V(\mathbf{r})}{\partial \phi}$

To prove the second relation, we have

$$[H, L^2] = \frac{1}{2m} [p^2, L^2] + [V(\mathbf{r}), L^2].$$
 ...(iii)

Now, p^2 commutes with L_z as shown above.

Similarly, it can be shown that it commutes with L_x and L_y . Thus p^2 will commute with L^2 . Hence from (iii), we have

$$[H, L^2] = [V(r), L^2].$$
 ...(iv)

For the central field, V will be a function of the radial distance r only and will be independent of θ and ϕ . Therefore, $\partial V/\partial \phi$ will vanish in (ii). Hence L_z commutes with H.

Similarly, L_x and L_y commute with H. Thus all the components of L commute with the Hamiltonian and hence L and any power of L will also commute with the Hamiltonian. L and all of its powers are the constants of motion for a central field problem.

Show that the operator L.S. has the eigenvalues \frac{1}{2} and -1 in the p-state of an electron. Also, derive the formula

$$L \cdot S = \frac{1}{2} (L_+ S_- + L_- S_+ + 2L_z S_z)$$

any verify directly that

L·S
$$|\frac{3}{2}, m\rangle = \frac{1}{2} |\frac{3}{6}, m\rangle$$
,
L·S $|\frac{1}{2}, m\rangle = -|\frac{1}{2}, m\rangle$.

and

Sol. For the p-state of an electron, the orbital angular momentum l=1. The spin of the electron $s=\frac{1}{2}$. Hence the total angular momentum J=L+S has the values from $(1+\frac{1}{2})$ to $|1-\frac{1}{2}|$ in integral steps, i.e. it has values $j=\frac{3}{2}$ and $\frac{1}{2}$.

Now
$$J^2 = (L+S)^2 = L^2 + S^2 + 2L.S.$$

 $L \cdot S = \frac{1}{2} (J^2 - L^2 - S^2)$

and

$$\langle \mathbf{L} \cdot \mathbf{S} \rangle = \frac{1}{2} \left[\langle J^2 \rangle - \langle L^2 \rangle - \langle S^2 \rangle \right]$$

$$= \frac{1}{2} \left[j (j+1) - l (l+1) - s (s+1) \right] \hbar^2$$

$$= \frac{1}{2} \left[j (j+1) - 1 \cdot (1+1) - \frac{1}{2} + 1 \right] \hbar^2$$

$$= \begin{cases} \frac{1}{2} \hbar^2 \text{ for } j = \frac{3}{2}, \\ -\hbar^2 \text{ for } j = \frac{1}{2}, \end{cases} \dots (i)$$

i.e. the eigen values of L.S are $\frac{1}{2}$ and -1.

The prove that $L \cdot S = \frac{1}{2} (L_+ S_- + L_- S_+ + 2L_z S_z)$, we get $L \cdot S = L_x S_x + L_y S_y + L_z S_z$

$$= \frac{1}{2} (L_{+} + L_{-}) \cdot \frac{1}{2} (S_{+} + S_{-}) + \frac{1}{2i} (L_{+} - L_{-}) \cdot \frac{1}{2i} (S_{+} - S_{-}) + L_{z} S_{z}$$

$$= \frac{1}{4} (L_{+} S_{+} + L_{+} S_{-} + L_{-} S_{+} + L_{-} S_{-})$$

$$- \frac{1}{4} (L_{+} S_{+} - L_{+} S_{-} - L_{-} S_{+} + L_{-} S_{-}) + L_{z} S_{z}$$

$$= \frac{1}{2} (L_{+} S_{-} + L_{-} S_{+} + 2L_{z} S_{z}) \cdot ... (ii)$$

$$= \frac{1}{2} (I_{+} S_{-} + I_{-} S_{-} + I_{-} S_{-}) + I_{z} S_{z}$$

$$= \frac{1}{2} (I_{+} S_{-} + I_{-} S_{+} + 2L_{z} S_{z}) \cdot ... (ii)$$

Using (ii) it can very easily be seen that

 $L \circ S \mid \frac{3}{2}, m \rangle = \frac{1}{2} \mid \frac{3}{2}, m \rangle$ $L \cdot S \mid \frac{1}{2}, m \rangle = - \mid \frac{1}{2}, m \rangle.$

and

Problem 3. The operator $S_r = \frac{S \cdot r}{r}$ is the component of the electron spin in the direction of the vector r. Since Sr is a scalar

perator, it commutes with each components of the total angular nomentum J=L+S, hence $[J, S_r]=0$.

Verify this by calculating $[L, S_r]$ and $[S, S_r]$ by means of the ommutation rules for L and r, i.e. show that

$$[S, S_r] = -[L, S_r] = i\hbar \frac{\mathbf{r} \times \mathbf{S}}{r}.$$
Sol. $[L, S_r] = \left[S, \frac{\mathbf{S} \cdot \mathbf{r}}{r}\right] = \frac{1}{r} \left[\hat{\mathbf{i}} L_x + \hat{\mathbf{j}} L_y + \hat{\mathbf{k}} L_z, S \cdot \mathbf{r}\right].$...(i)

Now, $[L_x, S_x] = [L_x, S_x \cdot x + S_y \cdot y + S_z \cdot z]$

$$= [L_x, S_y \cdot y] + [L, S_z \cdot z]$$

$$= S_y \left[L_x, y\right] + S_z \left[L_x, z\right]$$

$$= i\hbar S_y \cdot z - i\hbar S_z \cdot y$$

$$= -i\hbar (\mathbf{r} \times \mathbf{S})_x.$$
Similarly, $[L_y, S_x] = -i\hbar (\mathbf{r} \times \mathbf{S})_y$
and

Similarly,

 $[L_z, S.r] = -i \hat{n} (r \times S)_z$.

Equation (i) gives

$$[\mathbb{L}, S_r] = \frac{-i\hbar}{r} (r \times S). \qquad \dots (ii)$$

It can also be seen easity that

$$[S, S_r] = i\hbar \frac{(r \times S)}{r}$$
. ...(iii)

From (ii) and (iii), we have

or
$$[S, S_r] = -[L, S_r]$$
or
$$[S, S_r] \dotplus [L, S_r] = 0$$
or
$$[S \dotplus L, S_r] = 0$$
or
$$[J, S_r] = 0.$$

Problem 4. Prove that

$$L \times r - i\hbar r = i\hbar r - r \times L \equiv K$$
 (say) ...(i)

and show that this operator is Hermitian. also show that

$$[L^2, \mathbf{r}] = -2i\hbar\mathbf{K} \qquad ...(ii)$$

Sol. Let us take the x-component of the left hand side of (i) $(L \times r - i\hbar r)_x = (L_y z - L_z y) - i\hbar x$

$$= (L_y z - L_z y) - i \hbar x + (y L_z - z L_y) - (y L_z - z L_y)$$

$$= (L_y z - z L_y) + (y L_z - L_z y) - i \hbar x - (y L_z - z L_y)$$

$$= i \hbar x + i \hbar x - i \hbar x - (\mathbf{r} \times \mathbf{L})_x$$

$$= (i \hbar \mathbf{r} - \mathbf{r} \times \mathbf{L})_x.$$

Similarly, we can show that the y-and z-components of the left hand side are equal to the y-and z-components of the right hand side.

Since all the operators L and r appearing in K are Hermitian, therefore, K is Hermitian.

In order to calculate the commutator $[L^2, \mathbf{r}]$, we first calculate the x-component of it, viz.

$$\begin{split} [L^2, \, x] &= [L_x^2 + L_y^2 + L_z^2, \, x] = [L_y^2, \, x] + [L_z^2 \, x] \\ &= L_y \, [L_y, \, x] + [L_y, \, x] \, L_y + L_z \, [L_z, \, x] + [L_z, \, x] \, L_z \\ &= -i \hbar L_y z - i \hbar z L_y + i \hbar L_z y + i \hbar y L_z \\ &= i \hbar \, \left[(y L_z - z L_y) - (L_y z - L_z y) \right] \\ &= i \hbar \, \left[(\mathbf{r} \times \mathbf{L})_x - (\mathbf{L} \times \mathbf{r})_x \right]. \end{split}$$

From (i), we have

$$(\mathbf{r} \times \mathbf{L})_x = -K_x + i\hbar x$$
 and $(\mathbf{L} \times \mathbf{r})_x = K_x + i\hbar x$.

$$\vdots \quad [(\mathbf{r} \times \mathbf{L})_x - (\mathbf{L} \times \mathbf{L})_x] = -2K_x$$

$$[L^2, x] = -2i\hbar K_x.$$

and

Similarly,
$$[L^2, y] = -2i\hbar K_y$$
 and $[L^2, z] = -2i\hbar K_y$
Hence, $[L^2, \mathbf{r}] = -2i\hbar K$.

Problem 5. Prove the validity of the following commutation rules:

- (a) $[L_i, x_k] = i \hbar \epsilon_{ikl} x_l$,
- (b) $[L_i, p_k] = i \hbar \epsilon_{ik} p_i$ and
- (c) $[L_i, L_k] = i\epsilon_{ikl}L_l$.

[Hint: ϵ_{ikl} is the totally antisymmetrical tensor:

Using this definition of ϵ_{ikl} and the commutation relations between various components of L, r and p, the commutation relations (a), (b) & (c) can easily be verified.

Problem. 6. Obtain expression for the operators L_x , L_y , L_z in spherical coordinates by starting from the fact that L is related to infinitesimal rotation operators.

Sol. Let us first consider an infinitesimal rotation ϵ_z about the z-axis. This will change

$$x \to x' = x - \epsilon_z y,$$

$$y \to y' = \epsilon_z x + y$$

$$z \to z' = z.$$

and

Since 'z' remains unchanged.

$$0 = \delta z = \delta (r \cos \theta) = -r \sin \theta \ \delta \theta \Rightarrow \delta \theta = 0$$

 $\{: r \text{ is unchanged under any rotation}\}.$

Also,
$$-\epsilon_z y \equiv \delta x = \delta \ (r \sin \theta \cos \phi)$$

 $= r \cos \theta \ \delta \theta \cos \phi - r \sin \theta \sin \phi \ \delta \phi$
 $= -y \ \delta \phi \quad \{ : \delta \theta = 0 \text{ and } r \sin \theta \sin \phi = y \}$
 $\Rightarrow \epsilon_z = \delta \phi.$

Thus, under the above rotation

$$\theta \rightarrow \theta' = \theta,$$

 $\phi \rightarrow \phi' = \phi - \delta \phi$

and, therefore

$$\psi(r, \theta, \phi) \rightarrow \psi(r, \theta', \phi') = \psi(r, \theta, \phi - \delta\phi)$$

$$= \psi(r, \theta, \phi) - \delta\phi \frac{\partial\psi}{\partial\phi} \qquad \dots (i)$$

where we have neglected the square and higher powers of $\delta\phi$.

Also, the infinitesimal rotation matrix,

$$U_{z} = \left(I - \frac{i \epsilon_{z}}{\hbar} L_{z} \right) = \left(I - \frac{i \delta \phi}{\hbar} L_{z} \right) \{ : \epsilon_{z} = \delta \phi \}$$

$$\psi(r, \theta', \phi) = \left(I - \frac{i \delta \phi}{\hbar} L_{z} \right) \psi(r, \theta, \phi)$$

$$= \psi(r, \theta, \phi) - \frac{i \delta \phi}{\hbar} L_{z} \psi(r, \theta, \phi) \quad \dots \text{(ii)}$$

Comparing (i) and (ii) we see that

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

To find the expression for L_y , we consider an infinitesimal rotation ϵ_y about the y-axis. We have that

$$x \to x' = x - \epsilon_y z$$

$$y \to y' = y$$

$$z \to z' = \epsilon_y x + z$$

$$\epsilon_y x = \delta z = \delta(r \cos \theta) = -r \sin \theta \, \delta \theta$$

$$r \sin \theta \cos \phi \, \epsilon_y = -r \sin \theta \, \delta \theta$$

$$\Rightarrow \delta \theta = -\cos \phi \, \epsilon_y$$

Also we have

.. 7

or

 $0 = \delta y = \delta (r \sin \theta \sin \phi) = r \cos \theta \delta \theta \sin \phi + r \sin \theta \cos \phi \delta \phi$ or $-r \cos \theta \cos \phi \epsilon_y \sin \phi + r \sin \theta \cos \phi \delta \phi = 0$ $\Rightarrow \delta \phi = \cot \theta \sin \phi \epsilon_y$

$$\left(1 - \frac{i \epsilon_{y}}{\hbar} r_{y}\right) \psi(r, \theta, \phi) = \psi(r, \delta + \delta \theta, \phi + \delta \phi)$$

$$= \psi(r, \theta - \cos \phi \epsilon_{y}, \phi + \cot \theta \sin \phi \epsilon_{y})$$

$$= \psi(r, \theta, \phi) - \cos \phi \epsilon_{y} \frac{\partial \psi}{\partial \theta} + \cot \theta \sin \phi \epsilon_{y} \frac{\partial \psi}{\partial \phi}$$

$$\Rightarrow L_{y} = i \hbar \left[-\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi}\right]$$

Similarly, by considering an infinitesimal rotation about the x-axis we can show that

$$L_x = i \ln \left[\sin \theta \, \frac{\partial}{\partial \theta} + \cot \theta \, \cos \phi \, \frac{\partial}{\partial \phi} \right]$$

Problem 7. Obtain an expression for the operator of the orbital angular momentum relative to an arbitrary axis in \mathbb{R} rms of the operators $L_x L_y$ and L_z Hence show that the average value of the angular momentum relative to an axis making an angle θ with the z-axis is $(m \cos \theta)$.

Sol. Let the arbitrary axis be in the direction of the unit vector \hat{n} . Hence the direction cosines of this axis are:

 $\cos(\hat{i}, \hat{n})$; $\cos(\hat{j}, \hat{n})$ and $\cos(\hat{k}, \hat{n})$

and therefore, the components of the angular momentum operator $L_{\hat{n}}$ relative to the axis \hat{n} are given by:

$$(L_{\hat{n}})_{x} = L_{x} \cos(\hat{i}, \hat{n})$$
$$(L_{\hat{n}})_{y} = L_{y} \cos(\hat{j}, \hat{n})$$

and

$$(L_{\hat{n}})_z = L_z \cos(\hat{k}, \hat{n})$$

Thus,

$$\overrightarrow{L}_{\hat{n}} = \hat{i} \ L_x \cos(\hat{i}, \hat{n}) + \hat{j} \ L_y \cos(\hat{j}, \hat{n}) + \hat{k} \ L_z \cos(\hat{k}, \hat{n})$$

It is the required expression.

The second part of the problem can be visualised as follows. The momentum vector in any state Y_l^m is evenly "spread out" over a cone with its axis along the z-axis, its slant height equal to $\sqrt{l[(l+1)]}$, and its height equal to m. The average value of its projection on the xy-plane is equal to zero, and its component along the axis making an angle θ with the z-axis is, after averaging equal to $(m \cos \theta)$.

Problem 8. Consider a system of one kind of non-interacting particles. Let their momentum be the same and their spin be equal $to \frac{1}{2}$. If these particles did not possess spin we could describe the system by "pure case" ensemble. However, we do not know whether the spins of all the particles are parallel.

Is it possible to use an experiment of the Stern-Gerlack type to determine whether this beam of particles corresponds to a "pure case" or to a "mixture" ensemble?

Sol. It is possible. In the case of a mixed ensemble for every direction of the inhomogeneous magnetic field we shall always get a splitting into two beams. In the case of a pure ensemble by a suitable alignment of the instrument we can obtain the disappearance of one of the beams.

Problem 9. If A and B are two operators which commute with

o's, then show that

$$(A \circ \sigma) (B \circ \sigma) = (A \circ B) + i \sigma \circ (A \times B)$$

Use this result to show that

$$e^{i\overrightarrow{\theta}\overrightarrow{\sigma}.\hat{n}} = \cos\theta + i\overrightarrow{\sigma}.\hat{n}\sin\theta$$

where n is a unit vector in an direction.

Sol.

$$\overrightarrow{(A \circ \sigma)}(\overrightarrow{B} \circ \sigma) = (A_x \sigma_x + A_y \sigma_y + A_z \sigma_z)(B_x \sigma_x + B_y \sigma_y + B_z \sigma_z)
= A_x B_x + A_y B_y + A_z B_z + \sigma_x \sigma_y (A_x B_y - A_y B_x)
+ \sigma_y \sigma_z (A_y B_z - A_z B_y) + \sigma_z \sigma_x (A_z B_x - A_x B_z) ...(i)$$

"ORBITAL AND SPIN ANGULAR MOMENTA"

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In writing (i) we have used the relations

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$$
; $\sigma_x \sigma_y = -\sigma_y \sigma_x$ etc.

and the fact that A, B commutes with σ 's. We can now write (i) as:

$$(\overrightarrow{A} \cdot \overrightarrow{\sigma})(\overrightarrow{B} \cdot \overrightarrow{\sigma}) = \overrightarrow{A} \cdot \overrightarrow{B} + i \sigma_z (\overrightarrow{A} \times \overrightarrow{B})_z + i \sigma_x (\overrightarrow{A} \times \overrightarrow{B})_x$$

$$+ i \sigma_y (\overrightarrow{A} \times \overrightarrow{B})_y \quad \{ :: \quad \sigma_x \sigma_y = i \sigma_z \text{ etc.} \}$$
or
$$(\overrightarrow{A} \cdot \overrightarrow{\sigma})(\overrightarrow{B} \cdot \overrightarrow{\sigma}) = \overrightarrow{A} \cdot \overrightarrow{B} + i \overrightarrow{\sigma} \cdot (\overrightarrow{A} \times \overrightarrow{B}) \qquad \dots (ii)$$
which is the required result.

To prove the second part of the problem, we expand the exponential in a power series as:

$$e^{i\overrightarrow{\theta}} \circ \hat{n} = 1 + \frac{i \overrightarrow{\theta} \circ \hat{n}}{1!} + \frac{i^2 \theta^2 (\overrightarrow{\sigma} \circ \hat{n})(\overrightarrow{\sigma} \circ \hat{n})}{2!} + \frac{i^3 \theta^3 (\overrightarrow{\sigma} \circ \hat{n})(\overrightarrow{\sigma} \circ \hat{n})(\overrightarrow{\sigma} \circ \hat{n})(\overrightarrow{\sigma} \circ \hat{n})}{3!} + \dots$$

Using (i) with $A=B=\hat{n}$ in the above, we can write it as:

$$e^{i \theta \overrightarrow{\sigma} \hat{n}} = 1 + \frac{i \theta \overrightarrow{\sigma} \cdot \hat{n}}{1!} - \frac{6^{2} (1 + i \overrightarrow{\sigma} \cdot (\hat{n} \times \hat{n}))}{2!}$$

$$= \frac{i 6^{3} (\overrightarrow{\sigma} \cdot \hat{n})(1 + i \overrightarrow{\sigma} \cdot (\hat{n} \times \hat{n}))}{3!}$$

$$+ \dots \{ \therefore \hat{n} \cdot \hat{n} = 1 \}$$

$$= \left(1 - \frac{6^{2}}{2!} + \dots \right) + (i \sigma \cdot \hat{n}) \left(\frac{\theta}{1!} - \frac{6^{3}}{3!} + \dots \right)$$

$$\{ \therefore \hat{n} \times \hat{n} = 0 \}$$

$$= \cos \theta + i \overrightarrow{\sigma} \cdot \hat{n} \sin \theta.$$

$$(1 + i \overrightarrow{\sigma} \cdot (\hat{n} \times \hat{n}))$$

$$= \frac{1}{2!} + \dots + \frac$$

Problem 10. Find the eigenvalues and the eigenvectors for the operators S_x , S_y , S_z , in the representation by Pauli's matrices in which S_z is diagonal.

Sol. In Pauli's matrices representation we have (omitting \hbar) $S_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, S_x = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \text{ and } S_y = \begin{pmatrix} 0 & -i/2 \\ i/2 & 0 \end{pmatrix}$

To obtain the eigenvectors of S_x , we solve the matrix eigenvalue equation

$$\begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \lambda \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$$

The solutions are easily found to be:

$$\alpha s_x = \frac{1}{\sqrt{(2)}} e^{i\alpha_1} \begin{pmatrix} 1\\1 \end{pmatrix} \text{ for } \lambda = +\frac{1}{2}$$

$$\beta s_x = \frac{1}{\sqrt{(2)}} e^{i\beta_1} \begin{pmatrix} 1\\-1 \end{pmatrix} \text{ for } \lambda = -\frac{1}{2} \qquad \dots (i)$$

and

Similarly, for S_y and S_z we have :

Similarly, for by and
$$s_z$$
 we have .

$$\alpha s_y = \frac{1}{\sqrt{(2)}} e^{i\alpha_2} {1 \choose i} \text{ for } \lambda = +\frac{1}{2}$$
and
$$\beta s_y = \frac{1}{\sqrt{(2)}} e^{i\beta_2} {1 \choose -i} \text{ for } \lambda = -\frac{1}{2} \qquad ...(ii)$$
and
$$\alpha s_z = e^{i\gamma_3} {1 \choose 0} \text{ for } \lambda = +\frac{1}{2}$$
and
$$\beta s_z = e^{i\beta_3} {0 \choose 1} \text{ for } \lambda = -\frac{1}{2} \qquad ...(iii)$$

 α 's and β 's in the above are arbitrary phase factors.

Problem 11. Find the matrices corresponding to the spin operator components S_x , S_y , S_z for a particle of spin s=1 in the representation in which the operators S^2 and S_z are diagonal.

Sol. In a manner exactly similar to that for $s=\frac{1}{2}$, it can be shown here that:

$$S_{x} = \frac{1}{\sqrt{(2)}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; S_{y} = \frac{1}{\sqrt{(2)}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$S_{z} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \text{ and } S^{2} = 2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Problem 12. Show that the operator $S_{12}=2\left[3\frac{(S.r)^2}{r^2}S^2\right]$,

regarded as a function of \mathbf{r} , depends only on the polar angles θ and ϕ , and that this dependence has the form of a spherical harmonic with l=2.

Sol. In spherical polar coordinates, $\mathbf{r} = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)$, we have $S_x \cos \phi + S_y \sin \phi = \frac{1}{2} (S_+ e^{-i\phi} + S_- e^{i\phi})$ $\frac{1}{r^2} (S_- \mathbf{r})^2 = \left[\frac{1}{2} (S_+ e^{-i\phi} + S_- e^{i\phi}) \sin \theta + S_z \cos \theta\right]^2$ $= \frac{1}{4} S_+^2 e^{-2i\phi} \sin^2\theta + \frac{1}{4} S_-^2 e^{2i\phi} \sin^2\theta + \frac{1}{2} (S_+ S_z + S_z S_+)$ $+ e^{-i\phi} \sin \theta \cos \theta + \frac{1}{2} (S_- S_z + S_z S_-) e^{i\phi} \sin \theta \cos \theta$ $+ S_z^2 \cos^2\theta + \frac{1}{4} (S_+ S_- + S_- S_+) \sin^2\theta.$

Using the relations

$$[S_+, S_-] = 2 S_z$$
, $S^2 = S_+ S_- + S_z^2 - S_z$, $S_+ S_- + S_- S_+ = 2S_+ S_- - 2S_z$
= 2 $(S^2 - S_z^2)$ we get

$$S_{12} = \frac{3}{2} S_{+}^{2} e^{-2i\phi} \sin^{2}\theta + 3 \left(S_{+}S_{z} + S_{z}S_{+} \right) e^{-i\phi} \sin\theta \cos\theta - \left(3 S_{z}^{2} - S^{2} \right) \left(1 - 3 \cos^{2}\theta \right) + 3 \left(S_{-}S_{z} + S_{z}S^{+} \right) e^{i\phi} \sin\theta \cos\theta + \frac{3}{2} S_{-}^{2} e^{2i\phi} \sin^{2}\theta.$$

In terms of the spherical harmonics, with l=2, we find that:

$$S_{12} = \sqrt{\left(\frac{24\pi}{5}\right)} \left[S_{+}^{2} Y_{2}^{-2} + \left(S_{+} S_{z} + S_{z} S_{+}\right) Y_{2}^{-1} + \sqrt{\left(\frac{2}{3}\right)} \left(3S_{z}^{2} - S^{2}\right) Y_{2}^{0} - \left(S_{-} S_{z} + S_{z} S_{-}\right) Y_{2}^{1} + S^{2} - Y_{2}^{2}\right]}$$

Problem 13. Show that $\langle J_x \rangle = \langle J_y \rangle = 0$. and $\langle J_x^2 \rangle = \langle J_y^2 \rangle = \frac{1}{2} \hbar^2 \left[j (j+1) - \tilde{m}^2 \right]$ in a representation in which the operators J^2 and J_4 are diagonal.

Sol. We have

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$$J_x = \frac{1}{2} (J_+ + J_-)$$
 and $J_y = \frac{1}{2i} (J_+ - J_-)$

$$\therefore \langle J_x \rangle = \frac{1}{2} \left\{ \langle J_+ \rangle + \langle J_- \rangle \right\} \text{ and } \langle J_y \rangle = \frac{1}{2i} \left\{ \langle J_+ \rangle - \langle J_- \rangle \right\}$$

Now
$$\langle J_+ \rangle = \langle jm \mid J_+ \mid jm \rangle$$

$$=[(j-m)(j+m+1)]^{1/2}$$
 $(jm | j, m+1)=0$,

due to orthogonality of the angular momentum states | jm>.

Similarly, $\langle J_{-}\rangle = 0$; and hence, $\langle J_{x}\rangle = \langle J_{y}\rangle = 0$.

$$J_x^2 = \frac{1}{6} (J_+ J_+ + J_+ I_- + J_- J_+ + J_- J_-)$$

$$: \langle J_x^2 \rangle = \frac{1}{4} \left\{ \langle J_+ J_+ \rangle + \langle J_+ J_- \rangle + \langle J_- J_+ \rangle + \langle J_- J_- \rangle \right\}.$$

Now
$$\langle J_{+}J_{+}\rangle = \langle jm \mid J_{+}J_{+} \mid jm\rangle$$

 $= [(j-m)(j+m+1)]^{1/2}\hbar \langle jm \mid J_{+} \mid j, m+1\rangle$
 $= [(j-m)(j+m+1)]^{1/2}\hbar \cdot [(j-m-1)(j+m+1+1)]^{1/2}\hbar \langle jm \mid j, m+2\rangle$

Similarly, $\langle J_{-}J_{-}\rangle = 0$;

=0

$$\langle J_{+}J_{-}\rangle = \langle jm \mid J_{+}I_{-} \mid jm \rangle$$

$$= [(j+m)(j-m+1)]^{1/2} \hbar \langle jm | J_{+} | j, m-1 \rangle$$

=
$$[(i+m)(j-m+1)]^{1/2}$$
ħ $[(j-m+1)(j+m-1+1)]^{1/2}$ ħ

=
$$(j+m)(j-m+1) h^2$$

and $\langle J_-J_+\rangle = (j-m)(j+m+1) h^2$.

Hences,

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$$\langle J_x^2 \rangle = \frac{1}{4} \ln^2 \left[(j+m)(j-m+1) + (j-m)(j+m+1) \right]$$

 $= \frac{1}{2} \ln^2 \left[j (j+1) - m^2 \right]$

 $\langle jm \mid jm \rangle$

Exactly in a similar manner,

$$\langle J_{y}^{2} \rangle = \frac{1}{2} \hbar^{2} [j(j+1) - m^{2}].$$

Problem 14. Suppose the total angular momentum of a system $J = J_1 + J_2$. Show that

Sol.
$$J^2 >= [j_1 (j_1+1)+j_2 (j_2+1)+2m_1m_2] \hbar^2$$
.
Sol. $J^2 = J_1^2 + J_2^2 + 2 (J_{1x} J_{2x} + J_{1y} J_{2y} + J_{1z} J_{2z})$
 $\therefore \langle J^2 \rangle = \langle J_1^2 \rangle + \langle J_2^2 \rangle + 2 \{\langle J_{1x} J_{2x} \rangle + \langle J_{1y} J_{yy} \rangle + \langle J_{1z} J_{2z} \rangle\}$.
Now, $\langle J_1^2 \rangle = j_1 (j_1+1) \hbar^2$;
 $\langle J_2^2 \rangle = j_2 (j_2+1) \hbar^2$,
 $\langle J_{1x} J_{2x} \rangle = \langle J_{1x} \rangle \langle J_{2x} \rangle = 0$ (due to previous prob.)
 $\langle J_{1y} J_{2y} \rangle = \langle J_{1y} \rangle \langle J_{2y} \rangle = 0$ (due to previous prob.)

Using these, the required result follows at once.

 $\langle J_{1z}J_{2z}\rangle = \langle J_{1z}\rangle \langle J_{2z}\rangle = m_1\hbar m_2\hbar.$

Problem 15. Prove that every matrix representative of a component of a vector **J** which satisfies

$$J \times J = i J$$

has zero trace.

Sol. The components of J are given by

$$J_x = -i (J_y J_z - J_z J_y),$$

$$J_y = -i (J_z J_x - J_x J_z)$$

$$J_z = -i (J_x J_y - J_y J_x).$$

and

Trace
$$J_x = -i$$
 [Trace $(J_y J_z)$ —Trace $(J_z J_y)$]
$$= -i [\text{Trace } (J_y J_z) - \text{Trace } (J_y J_z)]$$

$$= 0. \qquad \{\because \text{ Trace } AB = \text{Trace } BA\}$$

Similarly, Trace $J_y=0$ and Trace $J_z=0$.

Problem 16. Prove the identity

$$[J_x^2, J_y^2] = [J_y^2, J_z^2] = [J_z^2, J_x^2]$$
 ...(i)

and show that these commutators are all zero in states for which $j=0, \frac{1}{2}$ or 1.

Sol. We have $J^2 = J_x^2 + J_y^2 + J_z^2$.

:
$$J_y^2 = J^2 - J_x^2 - J_z^2$$

Hence,
$$[J_x^2, J_y^2] = [J_x^2, J^2 - J_x^2 - J_z^2]$$

 $= [J_x^2, J^2] - [J_x^2, J_x^2] - [J_x^2, J_z^2]$
 $= -[J_x^2, J_z^2]$
 $\{ : J_x \text{ commutes with } J^2 \text{ and } J_x]$
 $= [J_z^2, J_x^2].$...(ii)

Similarly, using the fact that J_y commutes with J^2 and J_y^2 , we can show that

$$[J_y^2, J_z^2] = [J_x^2, J_y^2].$$
 ...(iii)

From (ii) and (iii), we can see that (i) follows at once. The second part of the problem can be proved by finding the matrix representations for J_x^2 , J_y^2 and J_z^2 for j=0, $\frac{1}{2}$ and 1; respectively. It will be seen that the matrix commutators will vanish.

Problem 17. Show that if any operator commutes with two of the components of an angular momentum vector, it commutes with the third.

Sol. Any two components of the angular momentum are related to the third by the relation of the form

$$[J_x, J_y] = i \hbar J_z. \qquad ...(i)$$

If any operator 'A' (say) commutes with J_x and J_y , then from (i) it can easily be seen that it will commute with J_z also. Similar is the case for the other components.

Problem 18. For the electron moving in a central field of force show that the eigenfunctions of H, L^2 , L_z and σ_z can be found as the simultaneous eigenfunctions. Obtain the explicit form of the eigenfunctions.

Sol. For a central field, H_z L^2 , L_z and σ_z all commutes among themselves and hence their simultaneous eigenfunctions can be found out. To find these functions, we write the eigenvalue equation for H as

$$H\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{1}$$

We have written the function as a two-component spinor because the matrix σ_z is a 2×2 matrix for the electron and hence its eigenfunction should also have two components.

Equation(i) can be written as two equations

$$H\psi_1 = E\psi_1$$
 and $H\psi_2 = E\psi_2$(ii)

 ψ_1 and ψ_2 , which are the solutions for a central potential, can be written in the form

$$R_{nl}$$
 (r) Y_l^m (θ, ϕ) ,

where R_{nl} is the radial part of the solution and Y_{l}^{m} is the angular part.

The eigenvalues of σ_z are +1 or -1, corresponding to the spin up and spin down states of the electron, respectively.

For spin up state, we have

$$\sigma_z \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$
$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

or

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or

$$\begin{pmatrix} \psi_1 \\ -\psi_2 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \Rightarrow \psi_2 = 0.$$

$$\psi_{nim} (\uparrow) = \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix} = \begin{bmatrix} R_{ni} (\mathbf{r}) Y_{lm} (\theta, \phi) \\ 0 \end{bmatrix}. \dots (iii)$$

For spin down state, we have

$$\sigma_{z} \begin{pmatrix} \psi_{1} \\ \psi_{2} \end{pmatrix} = -\begin{pmatrix} \psi_{1} \\ \psi_{2} \end{pmatrix}$$

$$\begin{pmatrix} \psi_{1} \\ -\psi_{2} \end{pmatrix} = \begin{pmatrix} -\psi_{1} \\ -\psi_{2} \end{pmatrix} \Rightarrow \psi_{1} = 0.$$

$$\therefore \quad \psi_{nlm} (\downarrow) = \begin{bmatrix} 0 \\ R_{nl} (\mathbf{r}) Y_{lm} (\theta, \phi) \end{bmatrix} \qquad .. (iv)$$

(iii) and (iv) are the simultaneous eigen functions of H, L^2 , L_z and σ_z .

Problem 19. A spin $\frac{1}{2}$ particle moves in a central field of force. Find the wavefunction of this particle which is a simultaneous eigenfunction of the three commuting operators:

$$J_z=L_z+S_z$$
, L^2 and J^2 .

Sol. First of all we find the eigenfunctions of the operator J_z . the matrix for this operator can be written as

$$J_z = \begin{bmatrix} L_z + \frac{1}{2} & 0 \\ 0 & L_z - \frac{1}{2} \end{bmatrix}.$$

Since $L_z=-i\hbar \frac{\partial}{\partial \phi}$, the equation determining the eigenfunctions and eigenvalues of J_z is of the form

$$\begin{pmatrix} -i\hbar \frac{\partial}{\partial \phi} + \frac{1}{2} & 0 \\ 0 & -i\hbar \frac{\partial}{\partial \phi} - \frac{1}{2} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = m \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$
or
$$-i\hbar \frac{\partial \psi_1}{\partial \phi} + \frac{1}{2} \psi_1 = m\psi_1,$$

$$-i\hbar \frac{\partial \psi_2}{\partial \phi} - \frac{1}{2} \psi_2 = m\psi_2.$$

It follows that

 $\psi_1 = f_1(r, \theta) \exp \left\{ \frac{i}{\hbar} (m - \frac{1}{2}) \phi_r \right\}, \ \psi_2 = f_2(r, \theta) \exp \left\{ \frac{i}{\hbar} (m + \frac{1}{2}) \phi \right\},$ where f_1 and f_2 are arbitrary functions of r and θ and m is a half integer.

From all possible functions of the form

$$\begin{pmatrix}
f_1(r, \theta) \exp \left\{ \frac{i}{\hbar} (m - \frac{1}{2}) \phi \right\} \\
f_2(r, \theta) \exp \left\{ \frac{i}{\hbar} (m + \frac{1}{2}) \phi \right\} \end{pmatrix}$$

we select those which are at the same time eigenfunctions of the operator L^2 . Such functions are of the form

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} R_1 (r) Y_l^{m-1/2} (\theta, \phi) \\ R_2 (r) Y_l^{m+1/2} (\theta, \phi) \end{pmatrix} ...(i)$$
 ...(i)

Now we have to choose R_1 and R_2 such that (i) becomes eigenfunction of J^2 also. To do this we write the equation $J^2\psi=j$ (j+1) $\hbar^2\psi$ in matrix form

$$\begin{pmatrix} L^{2} + \frac{3}{4} + L_{z} & L_{x} - iL_{y} \\ L_{x} + iL_{y} & L^{2} + \frac{3}{4} - L_{z} \end{pmatrix} \begin{pmatrix} R_{1}(r) & Y_{l}^{m-1/2}(\theta, \phi) \\ R_{2}(r) & Y_{l}^{m+1/2}(\theta, \phi) \end{pmatrix}$$

$$= j(j+1) \begin{pmatrix} R_{1}(r) & Y_{l}^{m-1/2}(\theta, \phi) \\ R_{2}(r) & Y_{l}^{m+1/2}(\theta, \phi) \end{pmatrix}$$

and take into account the properties of the spherical harmonics

$$\begin{array}{ll} (L_x + iL_y) \ Y_l^m = \sqrt{\{(l+m+1) \ (l-m)\}} \ \hbar Y_l^{m+1}, \\ (L_x - iL_y) \ Y_l^m = \sqrt{\{(l-m+1) \ (l+m)\}} \ \hbar Y_l^{m-1}. \end{array}$$

It follows then from the matrix relation which we have written down that R_1 and R_2 must satisfy two homogeneous equations

$$[l (l+1)-j (j+1)+m+\frac{1}{4}] R_1+\sqrt{\{(l+\frac{1}{2})^2-m^2\}} R_2=0,$$

$$\sqrt{\{(l+\frac{1}{2})^2-m^2\}} R_1+[l (l+1)-j (j+1)-m+\frac{1}{4}] R_2=0.$$

In order that these equations can be solved, it is necessary that j is equal to $l+\frac{1}{2}$ or $l-\frac{1}{2}$. If we take $j=l+\frac{1}{2}$, we get

$$R_1(r) = \sqrt{(l + \frac{1}{2} + m)} R(r),$$

 $R_2(r) = \sqrt{(l - m + \frac{1}{2})} R(r)$

and thus

thus
$$\psi(l, j=l+\frac{1}{2}, m) = R(r) \left[\sqrt{\left(\frac{l+m+\frac{1}{2}}{2l+1}\right)} Y_{l}^{m-1/2}(\theta, \phi) \right] \\
\sqrt{\left(\frac{l-m+\frac{1}{2}}{2l+1}\right)} Y_{l}^{m+1/2}(\theta, \phi) \right]$$

Similarly, we get for $j=l-\frac{1}{2}$:

The factor $\frac{1}{\sqrt{(2l+1)}}$ follows from the normalization.

Problem 20. A system consists of two particles, one with angular momentum $l_1=1$, and the other with angular momentum $l_2=1$. The total angular momentum J can in that case takes on values l+1, l and l-1. Express the eigenfunctions of the operators J^2 and J_z in terms of the eigenfunctions of the square and the z-component of the angular momentum of the separate particles.

The wavefunction of the system, ψ (j, m), has the form of a sum of products of functions of separate particles,

f products of functions of separation
$$\psi_{m}(jm) = C_1 \psi_1^{(1)} \psi_{m-1}^{(2)} + C_0 \psi_0^{(1)} \psi_m^{(2)} + C_{-1} \psi_{m+1}^{(1)} \psi_{m+1}^{(2)} \dots (i)$$

where the lower index on the wavefunctions indicates the value of the angular momentum component.

The coefficients C_i can be determined from the equation

ients
$$C_i$$
 can be determined:
$$J^2 \psi(j, m) = j(j+1)\hbar^2 \psi(j, m). \qquad \dots (ii)$$

$$J^2 \psi(j, m) = j(j+1)\hbar^2 \psi(j, m). \qquad \dots (ii)$$

The wavefunctions of the first particle can be written conveniently in the form

$$\psi_{1} \stackrel{(1)}{=} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \psi_{0}^{(1)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \psi_{-1}^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The operator L_1 will be a 3×3 matrix

The operator
$$L_1$$
 will be a 3×3 index.
$$L_{1x} = \frac{1}{\sqrt{(2)}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; L_{1y} = \frac{1}{\sqrt{(2)}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

$$L_{1z} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and we find for the operator J^2 :

$$J^{2} = L_{1}^{2} + L_{2}^{2} + 2L_{1} L_{2}$$

$$= \begin{pmatrix} l (l+1) + 2 + 2L_{2z} & \sqrt{(2)} L_{2} - & 0 \\ \sqrt{(2)} L_{2+} & l (l+1) + 2 & \sqrt{(2)} L_{2} - \\ 0 & \sqrt{(2)} L_{2+} & l (l+1) + 2 - 2L_{2z} \end{pmatrix}$$

where $L_+ = L_x + iL_y$, $L_- = L_x - iL_y$,

If we use the properties of the operators L_+ and L_- ,

$$L_{+}\psi_{m} = \sqrt{\{(l-m)(l+m+1)\}} \ \hbar \psi_{m+1},$$

$$L_{-}\psi_{m} = \sqrt{\{(l+m)(l-m+1)\}} \ \hbar \psi_{m-1},$$

we find that equation (ii) leads to two equations,

$$[j(j+1)-l(l+1)-2m] C_1 = \sqrt{2} \sqrt{\{(l+m) l-m+1\}} C_0,$$

$$[j(j+1)-l(l+1)+2m] C_{-1} = \sqrt{2} \sqrt{\{(l+m+1) (l-m)\}} C_0$$

If we solve these equations we find for C(j, m):

$$\begin{bmatrix}
C_{1} (l+1, m) & C_{0} (l+1, m) & C_{-1} (l+1, m) \\
C_{1} (l, m) & C_{0} (l, m) & C_{-1} (l, m) \\
C_{1} (l-1, m) & C_{0} (l-1, m) & C_{-1} (l-1, m)
\end{bmatrix} = \begin{bmatrix}
\sqrt{\left\{\frac{(l+m) (l+m+1)}{2 (2l+1) (l+1)}\right\}} & \sqrt{\left\{\frac{(l+m+1) (l-m+1)}{(2l+1) (l+1)}\right\}} \\
-\sqrt{\left\{\frac{(l+m) (l-m+1)}{2 l (l+1)}\right\}} & \sqrt{\left\{\frac{(l+m) (l-m+1)}{2 (2l+1)}\right\}} \\
-\sqrt{\left\{\frac{(l-m) (l-m+1)}{2 (2l+1)}\right\}} & -\sqrt{\left\{\frac{(l+m) (l-m)}{2 (2l+1) (l+1)}\right\}} \\
\sqrt{\left\{\frac{(l+m+1) (l-m)}{2 l (l+1)}\right\}} & \sqrt{\left\{\frac{(l+m+1) (l-m)}{2 l (2l+1)}\right\}} \\
\sqrt{\left\{\frac{(l+m) (l+m+1)}{2 l (2l+1)}\right\}} & \sqrt{\left\{\frac{(l+m) (l+m+1)}{2 l (2l+1)}\right\}}
\end{bmatrix}$$

Since the matrix is orthogonal, its inverse is the same as its transposed matrix and therefore, each of the functions $\psi_1^{(1)}$ $\psi_{m-1}^{(2)}$

 $\psi_0^{(1)}$ $\psi_{m}^{(1)}$, $\psi_{-1}^{(1)}$ $\psi_{m+1}^{(2)}$ can be expressed as a linear combination of ψ (l+1, m), ψ (l, m), ψ (l-1, m) with coefficients which are in the columns of this matrix.

Problem 12. Show that between the simultaneous eigenvectors of the operators J^2 and J_z , there exist the following relations:

$$|j, \pm m\rangle = \sqrt{\left\{\frac{(j+m)!}{(2j)!(j-m)!}\right\}} (J_{\pm})^{j-m} |j, \pm j\rangle.$$

$$|j, \pm j\rangle = \sqrt{\left\{\frac{(j+m)!}{(2j)!(j-m)!}\right\}} (J_{\pm})^{j-m} |j, \pm m\rangle.$$
Sol We have (deleting \hbar)
$$J_{-}|j, m+1\rangle = \sqrt{\left\{j(j+1)-m(m+1)\right\}} |jm\rangle$$

$$= \sqrt{\left\{(j-m)(j+m+1)\right\}} |jm\rangle$$

$$= \sqrt{\left\{(j-m)(j+m+1)(j+m+2)\right\}} |j, m+1\rangle$$

$$= \sqrt{\left\{(j-m-1)(j-m)(j+m+1)(j+m+2)\right\}} |jm\rangle$$
and in general,
$$(J_{-})^{j-m} |jj\rangle = \sqrt{\left\{1, 2, ... (j-m-1)(j-m)(j+m+1) \times (j+m+2) ... (2j-1)(2j)\right\}} |jm\rangle$$

$$= \sqrt{\left\{\frac{(2j)!(j-m)!}{(j+m)!}\right\}} |jm\rangle$$

$$\Rightarrow |j, m\rangle = \sqrt{\left\{\frac{(j+m)!}{(2j)!(j-m)!}\right\}} (J^{-})^{j-m} |j, j\rangle.$$

Similarly we can derive the other three relations.

Problem 22. Show that in a representation in which J_x and J_z are real matrices, J_y is of the form $i \times (a \text{ real antisymmetric matrix})$.

(Hint. It can be shown easily by using the commutation relation

$$[J_z, J_x] = iJ_y.$$

$$\sim \sim \sim \sim \sim \sim \sim$$
As $[J_z, J_x] = J_zJ_x - J_xJ_z = J_x J_z - J_z J_x = [J_x, J_z]$

$$= -[J_z, J_z]\},$$

Problem 23. Since the components of the angular momentum operator do not commute, their simultaneous measurement is not possible. Show that in a state $|jm\rangle$ the greatest accuracy of measurement of the components J_x and J_y is obtained when |m|=j.

Sol. The uncertaintly in the angular momentum J_x is defined

Similarly,

Now
$$\langle J_y = \sqrt{\langle jm | J_y^2 | jm \rangle}$$
. ...(ii)

$$\langle J^2 \rangle = \langle jm | J^2 | jm \rangle = \hbar^2 j (j+1) = \langle J_x^2 \rangle + \langle J_y^2 \rangle + \langle J_z^2 \rangle$$

$$= (\triangle J_x)^2 + (\triangle J_z)^2 + m^2 \hbar^2$$

Therefore,

$$(\triangle J_x)^2 + (\triangle J_y)^2 = (j^2 + j - m^2)\hbar^2 \qquad \dots (iii)$$

From (iii), we see that minimum value of the combined uncertainties of J_x and of J_y is obtained when |m| = j.

Problem 24. A hydrogen atom is in the p-state $(l=1, s=\frac{1}{2})$. Obtain the wavefunctions in terms of the spherical harmanics and the spin states.

Sol. Let us take $j_1=l=1$ and $j_2=s=\frac{1}{2}$.

Hence the state of the atom can be written as
$$|jm\rangle = \psi_{jm}$$
...(i)

Here j is the total angular momentum of the atom and m is its z-component.

Now, the states $|jm\rangle$ can be expanded in terms of the states $|j_1m_1\rangle$ and $|j_2m_2\rangle$ using the CG. coefficients as:

$$|jm\rangle = \sum |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | jm\rangle \dots (ii)$$

 m_1, m_2

where we have used the abbreviation

$$|j_1 j_2 m_1 m_2\rangle = |j_1 m_1 \otimes |j_2 m_2\rangle$$

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For $j_1=1, m_1=1, 0, -1$ and for $j_2=\frac{1}{2}, m_2=\frac{1}{2}$ and $-\frac{1}{2}$.

Possible $|j_1m_1\rangle$ states are $|1, 1\rangle, |1, 0\rangle$ and $|1, -1\rangle$ and $|j_2m_2\rangle$ states are $|\frac{1}{2}, \frac{1}{2}, \rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle$. j can take values from $|j_1-j_2|$ to j_1+j_2 i.e,

$$j = \frac{3}{2} & \frac{1}{2}$$

Corresponding to $j = \frac{3}{2}$, $m = \frac{3}{2}$, $\frac{1}{2}$, $-\frac{1}{2}$, $-\frac{3}{2}$ and corresponding to $j = \frac{1}{2}$, $m = \frac{1}{2}$ and $-\frac{1}{2}$.

 $\therefore \text{ Possible } |jm\rangle \text{ states are : } |\frac{3}{2}, \frac{3}{2}\rangle, |\frac{3}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, \frac{1}{2}\rangle, \\ |\frac{3}{2}, -\frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle \text{ and } |\frac{3}{2}, -\frac{3}{2}\rangle.$

Using (ii) and the values of C.G. coefficients for $j_1=1$ and $j_2=\frac{1}{2}$ we get:

$$\begin{vmatrix} \frac{3}{2}, \frac{3}{2} \rangle = |1, 1\rangle \otimes |\frac{1}{2}, \frac{1}{2} \rangle$$

$$\begin{vmatrix} \frac{3}{2}, \frac{3}{2} \rangle = \frac{1}{\sqrt{3}} |1, 1\rangle \otimes |\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \rangle + \sqrt{\frac{2}{3}} \times$$

$$|1, 0\rangle \oplus |\frac{1}{2}, \frac{1}{2} \rangle$$

$$\begin{vmatrix} \frac{1}{2}, \frac{1}{2} \rangle = \sqrt{\frac{2}{3}} |1, 1\rangle \otimes |\frac{1}{2}, -\frac{1}{2} \rangle - \frac{1}{\sqrt{3}} \times$$

$$|1, 0\rangle \otimes |\frac{1}{2}, \frac{1}{2} \rangle$$

$$\begin{vmatrix} \frac{3}{2}, -\frac{1}{2} \rangle = \sqrt{\frac{2}{3}} |1, 0\rangle \otimes |\frac{1}{2}, -\frac{1}{2} \rangle$$

$$+ \frac{1}{\sqrt{3}} |1, -1\rangle \otimes |\frac{1}{2}, \frac{1}{2} \rangle$$

$$\begin{vmatrix} \frac{1}{2}, -\frac{1}{2} \rangle = \frac{1}{\sqrt{3}} |1, 0\rangle \otimes |\frac{1}{2}, -\frac{1}{2} \rangle - \sqrt{\frac{2}{3}} \times$$

$$|1, -1\rangle \otimes |\frac{1}{2}, \frac{1}{2} \rangle$$

$$\begin{vmatrix} \frac{3}{2}, -\frac{3}{2} \rangle = |1, -1\rangle \otimes |\frac{1}{2}, -\frac{1}{2} \rangle$$

Now the wave-functions for the hydrogen atom can be written as:

$$\psi_{nlm} = R_{nl}(r) Y_l^m(\theta, \phi) \times \text{spin state}$$

where R_{nl} is the radial wavefunction and Y_l^m , s are the spherical harmonics. The spin up state $|\frac{1}{2}, \frac{1}{2}\rangle$ can be represented by the spinor $\binom{1}{0}$ and the spin down state $|\frac{1}{2}, -\frac{1}{2}\rangle$ can be represented by the spinor $\binom{0}{1}$. Thus we can write

$$\left|\begin{array}{c} \frac{3}{2}, \frac{3}{2} \right\rangle = R_{n_1}(r) Y_1^1(\theta, \phi) \begin{pmatrix} 1\\ 0 \end{pmatrix}$$

$$= \begin{bmatrix} R_{n_{1}}(r) & Y_{1}^{1} & (\theta, \phi) \\ 0 & 1 \end{bmatrix}$$

$$= \frac{1}{\sqrt{3}} R_{n_{1}}(r) & Y_{1}^{1} & (\theta, \phi) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$+ \sqrt{\frac{2}{3}} R_{n_{1}}(r) & Y_{1}^{0} & (\theta, \phi) \begin{pmatrix} \frac{1}{0} \end{pmatrix}$$

$$= \begin{bmatrix} \frac{1}{\sqrt{3}} R_{n_{1}}(r) & Y_{1}^{1} & (\theta, \phi) \\ \sqrt{\frac{2}{3}} R_{n_{1}}(r) & Y_{1}^{0} & (\theta, \phi) \end{bmatrix}$$

Similarly, we can write all the other states in terms of the spherical harmonics as a two component spinors.

Problem 25. Consider an electron with orbital angular momenum l and spin $\frac{1}{2}$. Under spin orbit interaction, the two possible alues of j are $l+\frac{1}{2}$ and $l-\frac{1}{2}$. Show that the expectation values of S_z in the state $j=l+\frac{1}{2}$ and $l-\frac{1}{2}$ are $\frac{m\hbar}{2l+1}$ and $-\frac{m\hbar}{2l+1}$ respectively.

Sol. Taking $j_1=l$ and $j_2=\frac{1}{2}$ we have $j=(j_1+j_2)$ to $|j_1-j_2|=l+\frac{1}{2}$ and $l-\frac{1}{2}$.

If the z-component of J has (2j+1) values (-j to +j) denoted y m, then we have the two sets of states for the electron as:

$$|jm\rangle \equiv |l+\frac{1}{2}, m\rangle$$
 and $|l-\frac{1}{2}, m\rangle$

The C.G. coefficient matrix for these states is given in the ollowing table:

$$\frac{j}{m_{1} m_{2}} \frac{l + \frac{1}{2}}{m} \qquad m$$

$$\frac{i - \frac{1}{2}}{2l} \frac{1}{2} \frac{1}{2} \frac{l + m + \frac{1}{2}}{2l + 1} - \sqrt{\frac{l - m + \frac{1}{2}}{2l + 1}}$$

$$\frac{l + \frac{1}{2}}{2l} - \frac{1}{2} \frac{l - m + \frac{1}{2}}{2l + 1} \frac{l - m + \frac{1}{2}}{2l + 1}$$

$$\frac{l + \frac{1}{2}}{2l}, m = \sqrt{\frac{l + m + \frac{1}{2}}{2l + 1}} \frac{m - \frac{1}{2}, \frac{1}{2}}{m - \frac{1}{2}, \frac{1}{2}}$$

$$+ \sqrt{\frac{l - m + \frac{1}{2}}{2l + 1}} \frac{m + \frac{1}{2}, -\frac{1}{2}}{2l + 1}$$

$$\langle S_{z} \rangle_{j = l + \frac{1}{2}} = \frac{l + m + \frac{1}{2}}{2l + 1} \frac{1}{2} \hbar + \frac{l - m + \frac{1}{2}}{2l + 1} - \frac{1}{2} \hbar$$

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$$=\frac{m\hbar}{2l+1}$$

Similarly,

$$\langle S_z \rangle = -\frac{m\hbar}{2l+1}$$

$$j = l - \frac{1}{2}$$

Problem 26. Use the C.G. coefficients for $j_1=j_2=\frac{1}{2}$ to write the spin states for two particles of spin $\frac{1}{2}$ and determine the nature of symmetry of these functions.

Sol. For $j_1=j_2=\frac{1}{2}$, we have j=1 & 0. Corresponding to $j_1=1$, m=1, 0, -1 and for j=0, m=0. Thus we have four $|jm\rangle$ states, viz, $|1, 1\rangle$, $|1, 0\rangle$, $|1, -1\rangle$ and $|0, 0\rangle$. Using the values of C.G. coefficients, these can be written in terms of the states $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ as:

$$|1, 1\rangle = \alpha x \qquad \dots (a)$$

$$|1,0\rangle = \frac{1}{\sqrt{2}} (\alpha\beta + \beta\alpha) \qquad ...(b)$$

$$|1, -1\rangle = \beta\beta \qquad ...(c)$$

and

$$|0,0\rangle = \frac{1}{\sqrt{2}} (\alpha \beta - \beta \alpha) \qquad \dots (d)$$

where we have used the notations:

re we have used the notations.

$$|j_1m_1\rangle \equiv |\frac{1}{2}, \frac{1}{2}\rangle = \alpha(\text{spin up}) \text{ and } |\frac{1}{2}, -\frac{1}{2}\rangle = \beta(\text{spin down})$$

 $|j_2m_2\rangle \equiv |\frac{1}{2}, \frac{1}{2}\rangle = \alpha(\text{spin up}) \text{ and } |\frac{1}{2}, -\frac{1}{2}\rangle = \beta \text{ (spin down)}$

When we interchange α and β in the above four states, we see that the states (a), (b) and (c) remains unchanged while the state (d) changes sign. Thus the first three states are symmetric and the last state is an antisymmetric state. The states with j=1is a triplet one while the state with j=0 is a singlet state.

Problem 27. Show that the operator $(\sigma_1, \sigma_2)^n$, where σ_1 and σ_2 are Pauli matrices, depends linearly on the product (σ_1, σ_2) . Find the explicit form of this dependence.

Sol. From the previous problem we see that if $j_1 = s_1 = \frac{1}{2}$ and $j_2 = s_2 = \frac{1}{2}$ are the spin values for two electrons, then (a), (b), (c) and (d) are the states of the combined system of the electrons. If S is the spin operator for the combined system, then

$$S=S_1+S_2$$

or
$$S^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2$$

$$(S_1, S_2) = \frac{1}{2} (S^2 - S_1^2 - S_2^2)$$

Hence,

$$(S_1.S_2) \mid 0, 0\rangle = -\frac{1}{2} (S_1^2 + S_2^2) \mid 0, 0\rangle$$

$$= -\frac{\hbar^2}{2} \left(\frac{3}{4} + \frac{3}{4} \right) \mid 0, 0\rangle$$

$$= -\frac{3\hbar^2}{4} \mid 0, 0\rangle$$

Now,
$$S = \frac{\hbar}{2} \xrightarrow{\sigma}$$
, therefore $(S_1, S_2) = \frac{\hbar^2}{4} \xrightarrow{\sigma} \xrightarrow{\sigma}$...(i)

Hence from (i) we have

$$\overrightarrow{(\sigma_1 \cdot \sigma_2)} \mid 0, 0 \rangle = -3 \mid 0, 0 \rangle \qquad \dots (ii)$$

Similarly, it can be shown that,

$$\begin{array}{c}
\overrightarrow{(\sigma_{1} \cdot \sigma_{2})} \mid 1, 1 \rangle = 1 \mid 1, 1 \rangle \\
\overrightarrow{(\sigma_{1} \cdot \sigma_{2})} \mid 1, 0 \rangle = 1 \mid 1, 0 \rangle \\
\overrightarrow{(\sigma_{1} \cdot \sigma_{2})} \mid 1, -1 \rangle = 1 \cdot \mid 1, -1 \rangle
\end{array} \dots (iii)$$

and

Thus we see that

From (iv) we can write,

$$\overrightarrow{(\sigma_1 \cdot \sigma_2)^n} \mid s = 0, \ l_z \rangle = (-3)^n \mid s = 0, \ s_z \rangle$$

$$\overrightarrow{(\sigma_1 \cdot \sigma_2)^n} \mid s = 1, \ s_z \rangle = |s = 1, \ s_z \rangle.$$

Since the three triplet states and the singlet state together form a complete orthonormal basis in the space of the spin states of two

electrons, it is sufficient to verify the linear dependence of $(\sigma_1, \sigma_2)^n$

on (σ_1, σ_2) for these states. Let us suppose then that

$$\overrightarrow{(\sigma_1 \cdot \sigma_2)^n} = C_1 \overrightarrow{(\sigma_1 \cdot \sigma_2)} + C_2 \qquad \dots (v)$$

where the coefficients C_1 and C_2 are to be determined. Applying both sides of the operator relation (v) to the triplet states and to the singlet state, we obtain

$$C_1+C_2=1$$
 and $-3C_1+C_2=(-3)''$

So that,

$$C_1 = \frac{1}{4}[1 - (-3)^n]$$
 and $C_2 = \frac{1}{4}[3 + (-3)^n]$

Note that for n=2

$$\overrightarrow{(\sigma_1} \cdot \overrightarrow{\sigma_2})^2 = -2(\overrightarrow{\sigma_1} \cdot \overrightarrow{\sigma_2}) + 3.$$

Problem 28. Show that for a system of two identical particles, each of spin s, the ratio of the number of symmetrical to the number of anti-symmetrical spin states is (s+1)/s.

Sol. Since for any of the particles there are possible (2s+1) spin orientations, the total number of independent spin functions for the system of the two particles is equal to $(2s+1)^2$.

These functions, which are not symmetrised with respect to the spins, have the form $\chi_i^{(l)}\chi_k^{(2)}$, where $i, k=-s, \ldots, s-1$, s. If we symmetrise them we get symmetric function of the form $\chi_i^{(1)} x_i^{(2)}$ for $i \neq k$, there are $(2s+1)^2 - (2s+1) = 2s (2s-1)$ functions of which one half, that is, s(2s+1) functions are of the form $(\chi_i^{(1)} \chi_k^{(2)} + \chi_k^{(1)} \chi_i^{(2)})$ (symmetrical) and s(2s+1) functions of antisymmetrical form

$$\left(\chi_{i}^{(1)} \ \chi_{k}^{(2)} - \chi_{k}^{(1)} \ \chi_{i}^{(2)}\right)$$

In this way we get altogether (s+1)(2s+1) functions which are symmetric w.r.t. permutations of the spins of the two particles and s(2s+1) antisymmetric functions which lead to the required ratio

$$\frac{s+1}{s}$$

Problem 29. Show that the transposition operators P_{ij} commutes with the Hamiltonian of a system of 'n' identical particles, while the operators P_{ij} do not commute with one another.

Sol. We illustrate it only for the system of three particles. The result can be generalized to 'n' particle system exacty in the same way.

$$P_{13} H (1, 2, 3) \psi (1, 2, 3) = H (3, 2, 1) \psi (3, 2, 1)$$

= $H (1, 2, 3) \psi (3, 2, 1)$...(i

we have written the last result from the fact that the Hamiltonian for a system of identical particle does not change by the interchange of the particles.

Also,
$$H(1, 2, 3)$$
 P_{13} $\psi(1, 2, 3) = H(1, 2, 3)$ $\psi(3, 2, 1)$...(ii)

From (i) and (ii) we see that

$$P_{13} H = H P_{13}$$

To illustrate the second part of the problem, let us consider

$$P_{13}$$
 P_{12} ψ (1, 2, 3)= P_{18} ψ (2, 1, 3)= ψ (3, 1, 2)
= P_{23} ψ (3, 2, 1)= P_{23} P_{13} ψ (1, 2, 3)

Thus

 $P_{23} P_{13} = P_{13} P_{12} \neq P_{12} P_{13}$

symmetrization and the anti-Problem 30. Show that the symmetrization operators are orthogonal projection operators; i,e., that $S^2 = S$, $A^2 = A$, SA = AS = 0.

and the antisymmetrization [Hint. The symmetrization operations are defined by:

$$S = \frac{1}{\sqrt{(n !)}} \Sigma P, A = \frac{1}{\sqrt{(n !)}} \Sigma (-1)^p P, \dots (i)$$

where the summation is to be taken over all n! permutation operators. Suppose that these operators have been placed in some particular order and we multiply them on the right (or on the left) by a given permutation operator P'. This will merely change the order in the arrangement of n! permutation operators. Owing to the summation in (i), it follows that

$$P'S = SP' = S, P'A = AP' = (-1)^{P'}A.$$
 ...(ii)

From (i) and (ii) the relations stated in the problem can easily be obtained.]

Problem 31. Write down the spin wavefunctions of proper symmetry for a system of two identical particles, each of spin 1.

[Hint. This prob. can be solved by using the C.G. coeffici-Taking the one particle states corresponding to $s_z=1$, 0 and -1 as α , β and γ ; respectively, the result is as given below:

Symmetrical States:

(i)
$$\alpha \alpha : s=2, s_z=2$$

(ii)
$$\frac{1}{\sqrt{(2)}} (\alpha \beta + \beta \alpha)$$
; $s=2$, $s_z=1$

(iii)
$$\sqrt{\left(\frac{2}{3}\right)} \left(\beta\beta + \frac{1}{2} \alpha\gamma + \frac{1}{2} \gamma\alpha\right)$$
; $s=2$, $s_z=0$.

(iv)
$$\frac{1}{\sqrt{(2)}} (\beta \gamma + \gamma \beta)$$
; $s=2$, $s_z=-1$.

(v)
$$\gamma \gamma$$
; $s=2$, $s_z=-2$.

(vi)
$$\frac{1}{\sqrt{3}} (\beta \beta - \alpha \gamma - \gamma \alpha)$$
; $s=0$, $s_z=0$.

Antisysmmetrial States:

(i)
$$\frac{1}{\sqrt{(2)}} (\alpha \beta - \beta \alpha)$$
; $s=1$, $s_z=1$

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(ii)
$$\frac{1}{\sqrt{(2)}} (\alpha \gamma - \gamma z)$$
; $s = 1, !s_z = 0$

(iii)
$$\frac{1}{\sqrt{(2)}}(\beta \gamma - \gamma \beta)$$
; $s=1$, $s_z=-1$.

Problem 32. Write down the normalized wavefunctions of a system of three identical bosons, which are in given one particle

Sol. Let $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ be the normalized one-particle states. states. We have now to distinguish three cases:

(a) All the three occupied states are different, i.e., $|\psi(1)\rangle \neq$ $|\psi(2)\neq |\psi(3)\rangle$. Then the state vector of the system will be

$$|\psi\rangle^{(s)} = S |\psi_{1}(1) \psi_{2}(2) \psi_{3}(3)\rangle$$

$$= \frac{1}{\sqrt{(3!)}} [|\psi_{1}(1) \psi_{2}(2) \psi_{3}(3)\rangle + |\psi_{1}(1) \psi_{2}(3) \psi_{3}(2)\rangle$$

$$+ |\psi_{1}(3) \psi_{2}(2) \psi_{3}(1)\rangle + |\psi_{1}(3) \psi_{2}(1) \psi_{3}(2)\rangle$$

$$+ |\psi_{1}(2) \psi_{2}(1) \psi_{3}(3)\rangle + |\psi_{1}(2) \psi_{2}(3) \psi_{3}(1)\rangle] ...(i)$$

(b) Two of the three filled states are identical, e.g. $|\psi(1)\rangle \neq |\psi(2)\rangle = |\psi(3)\rangle$. Then

$$|\psi\rangle^{(6)} = \sqrt{\left(\frac{2!}{3!}\right) \left[|\psi_{1}(1)|\psi_{2}(2)|\psi_{3}(2)\rangle + |\psi_{1}(2)|\psi_{2}(1)|\psi_{3}(2)\rangle + |\psi_{1}(2)|\psi_{2}(2)|\psi_{3}(1)\rangle \right]}.$$

(c) All three particles are in the same state; i.e., $|\psi(1)\rangle = |\psi(2)\rangle = |\psi(3)\rangle$ $|\psi\rangle^{(s)} = |\psi_1(1)|\psi_2(1)|\psi_3(1)\rangle.$

Problem 33. Express the operators r, p and L as irreducible tensor operators.

Sol. The components of the operators r, p and L satisfy the following commutation rules:

Tollowing commutation rules .
$$[L_i, x_k] = i\hbar \epsilon_{ikl} x_l ; [L_i, p_k] = i\hbar \epsilon_{ikl} p_l$$
and $[L_i, L_k] = i\epsilon_{ikl} L_l$.

Let A_x , A_y , A_z be the components of any vector operator, which is such that

$$[L_i, A_k] = i \epsilon_{ikl} A_l \qquad ...(ii)$$

where the indices 1, 2, 3 stands for the x-, y-and z-components as usual. Let us define the spherical components of A as:

$$A_1^{(1)} = -(A_x + iA_y)/\sqrt{2}$$
; $A_0^{(1)} = A_z$ and $A_{-1}^{(1)} = (A_x - iA_y)/\sqrt{2}$,

It can very easily be seen that,

$$\left[L_{\pm_{3}}A_{m}^{(1)}\right] = \sqrt{\{1\ (1+1)-m\ (m\pm1)\}}\,\,\hbar\,\,A_{m\pm1}^{(1)} \qquad ...(iii)$$

$$\begin{bmatrix} L_z, A_m^{(1)} \end{bmatrix} = m A_m^{(1)} \qquad \dots \text{(iv)}$$
For example,

For example,
$$\begin{bmatrix} L_1, A_0^{(1)} \end{bmatrix} = [L_1, A_3] + i [L_2, A_3] = -i \hbar A_2 - \hbar A_1 = \sqrt{2} A_1^{(1)}$$

Taking into account (iii), (iv) and the definition the irreducible tensor operators (eqns. 92) the problem is easily solved.

Problem 34. Find the matrix elements of the z-component of

the unit vector \hat{n} in the direction of r, for a spinless particle, in terms of the eigenfunctions of angular momentum of the particle.

Using the results of the above problem, we can write [Hint.

the components of the vector \hat{n} in terms of irreducible tensor operators, and thus the required matrix elements can be determined using Wigner Eckart theorem]

Problem 35. Let L be the orbital angular momentum of a spinless particle, and A an operator whose componetns satisfy the commutation rules:

$[L_i, A_k] = i \epsilon_{ikl} A_l$

Using the Winer Eckart theorem, find the matrix elements of the components of the operator A in the (L^2, L_z) representation.

Using the Wigner-Eckart theorem, we obtain the required matrix elements in the form:

$$\langle l_1, m_1 \mid A_{m_1}^{(1)} \mid l_2, m_2 \rangle = \langle l_1 \parallel A_{m_1}^{(1)} \parallel l_2 \rangle \langle l_2, 1, m_{22}, m \mid l_1 m_1 \rangle$$

where $A_{m}^{(1)}$ are the spherical components of A, and the expression $\langle l_1 \parallel A^{(1)} \parallel l_2 \rangle$ depends, for a given A, only on l_1 and l_2 .

In the following we shall require the C.G. coefficients $\langle l_2 l, m_2, m | l_1, m_1 \rangle$, given by equations (68).

Suppose first that m=-1. Then, since $m_2+m=m_1$ we obtain $m_2=m_1+1$. For l_2 we have three possibilities, viz, $l_1=l_2\pm 1$ or l_2 , so that, conversely, $l_2 = l_1 \mp 1$ or l_1 . Then we can write directly, for the non-vanishing matrix elements,

$$\langle l, m_{1} | A_{-1}^{(1)} | l_{1}-1, m_{1}+1 \rangle = a_{l_{1}, l_{1}-1}$$

$$\langle l_{1}=1, 1, m_{1}+1, -1 | l_{1}, m_{1} \rangle$$

$$= a_{l_{1}, l_{1}-1} \left[\frac{(l_{1}-m_{1}-1)(l_{1}-m_{1})}{(2l_{1}-1) 2l_{1}} \right]^{1/2}$$

where the coefficients a_{l_1} , $l_{1}-1 = \langle l_1 \parallel A^{(1)} \parallel l_1 - 1 \rangle$ are independent of m_1 , Similarly

$$= a_{l_1, l_1+1} \left[\frac{(l_1+m_1+2)(l_1+m_1+1)}{(2l_1+2)(2l_1+3)} \right]^{1/2};$$
For $m=0, m_2=m_1$

$$\langle l_1, m_1 \mid A_0^{(1)} \mid l_1-1, m_1 \rangle = a_{l_1, l_1-1} \left[\frac{(l_1-m_1)(l_1+m_1)}{l_1(2l_1+1)} \right]^{1/2};$$

$$\langle l_1, m_1 \mid (A_0^{(1)} \mid l_1, m_1) = a_{l_1, l_1} \frac{m_1}{[l_1(l_1+1)]^{1/2}};$$

and

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$$\langle l_1, m_1 | A_0^{(1)} | l_1+1, m_1 \rangle$$

$$= -a_{l_1, l_1+1} \left[\frac{(l_1-m_1+1)(l_1+m_1+1)}{(l_1+1)(2l_1+3)} \right]^{1/2};$$

The matrix element for m=+1 can also be obtained in the same way, using the relevent C.G. coefficients.

In the development of quantum mechanics, only a few simple physical problems like Hydrogen atom, harmonic oscillator and rigid rotator etc. could be solved completely and exactly. However in practice, exactly solvable problems are rare, i.e., for the majority of systems of physical interest, the exact solution of the Schroedinger equation presents great mathematical difficulties. In order to permit the discussion of these systems, various methods of approximate solutions of the wave equation have been devised, leading to more or less accurate approximate evaluation of energy values and wave-functions. Really speaking, there are as many approximation methods as there are problems and there is no question of treating them all here. In this book we present only three most general methods which are useful under different conditions.

8.1. PERTURBATION METHODS:

Out of these methods, a simple and beautiful one is wave mechanical perturbation theory daveloped by Schroedinger in 1926. If the problem at hand is sufficiently similar to one that has an exact solution, the Hamiltonian can be broken up into two parts, one of which is large and characterizes the system for which the Schroedinger equation can be solved exactly, while the other part is small and can be treated as a perturbation. Perturbation theories are of two kinds:

- (i) time-independent perturbation theory and
- (ii) time-dependent perturbation theory.

In the time-independent method, Hamiltonian does not depend on time, while in the time-dependent method Hamiltonian depends explicitly on time.

TIME-INDEPENDENT PERTURBATION THEORY FOR NON-DEGENERATE CASE:

Let us suppose that the discrete set of all the eigenvalues $E_{-}^{(0)}$ and the orthonormal set of eigenfunctions $\psi_n^{(0)}$ of the unperturbed Hamiltonian H(0) of a system are known,

$$H^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}, \dots (1)$$

in which $E_n^{(0)}$ is the energy of the nth level of the system with the corresponding state function as $\psi_n^{(0)}$. Now, if a small perturbation is added to the system so that the Hamiltonian changes to H, then the energy levels and the stationary states of the system are given by the solution of the eigenvalue equation

 $H\psi = E\psi$ Usulally this equation is not exactly soluble. The perturbation theory provides a systematic method of successive approximations to the eigenfunction ψ and the eigenvalue E in terms of the unperturbed eigenfunctions $\psi_n^{(0)}$ and eigenvalues $E_n^{(0)}$. The basic idea is to split up H into the unperturbed Hamiltonian $H^{(0)}$ plus a perturbation part H',

$$H = H^{(0)} + \lambda H',$$
 ...(3)

where the small parameter λ characterizes the strength of the perturbation*.

We now develop the perturbation theory assuming that E and ψ can be expressed as power series in λ such that the zero, the first. etc, powers of λ correspond to the zero, the first etc. orders of approximation,

$$\psi = \psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \dots$$

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots$$
(5)

Substituting Eqs. (4) and (5) in Eq. (2) and grouping the terms of the same order together, we have

$$\frac{e^2}{ch} \cong \frac{1}{137}$$

^{*}For example, when the unperturbed system is an atom, and the perturbation is due to electromagnetic field acting on it, the parameter λ is the fine

$$(H^{(0)}-E_0) \psi_0 + [(H^{(0)}-E_0) \psi_1 + (H'-E_1) \psi_0] \lambda + [(H^{(0)}-E_0) \psi_2 + (H'-E_1) \psi_1 - E_2 \psi_0] \lambda^2 + \dots = 0 \qquad \dots (6)$$

We want this equation to be valid for any arbitrary (but small) strength of the perturbation, i.e., for any value of λ . This can happen only if the co-efficient of each power of λ vanishes. Thus we should have

$$(H^{(0)}-E_0)\psi_0=0$$
 ...(7a)

$$(H^{(0)}-E_0) \psi_1=(E_1-H') \psi_0$$
 ...(7b)

$$(H^{(0)}-E_0) \psi_2=(E_1-H') \psi_1+E_2 \psi_0$$
 ...(7c)

etc. These are the zeroth order, first order, second order, ..., equations of the perturbation theory. The zeroth order equation (7a) means that ψ_0 is any one of the unperturbed eigenfunctions. Let us take

$$\psi_0 = \psi_m^{(0)}$$
 and $E_0 = E_m^{(0)}$...(8)

and suppose that $\psi_m^{(0)}$ is non-degenerate.

Evaluation of first-order energy E₁. Using eq. (8), we can write the first-order perturbation equation (7b) as:

$$(H^{(0)}-E_m^{(0)}) \psi_1=(E_1-H') \psi_m^{(0)}$$
 ...(9)

For the solution of this equation we expand ψ_1 in terms of the complete set of unperturbed wave functions $\psi_n^{(0)}$,

$$\psi_1 = \sum_{n=0}^{\infty} a_n^{(1)} \psi_n^{(0)} \dots (10)$$

$$H^{(0)}\psi_1 = \sum_{n} a_n^{(1)} H^{(0)} \psi_n^{(0)}$$

$$= \sum_{n}^{\infty} a_n^{(1)} E_n^{(0)} \psi_n^{(0)} \dots (11)$$

Substituting equations (10) and (11) into (9). we have

$$\sum_{n} a_{n}^{(1)} E_{n}^{(0)} \psi_{m}^{(0)} - E_{m}^{(0)} \sum_{n} a_{n}^{(1)} \psi_{n}^{(0)} = (E_{1} - H') \psi_{m}^{(0)}$$

or
$$\sum_{n} a_n^{(1)} (E_n^{(0)} - E_m^{(0)}) \psi_n^{(0)} = (E_1 - H') \psi_m^{(0)}$$
 ...(12)

Multiplying equation (12) by $\psi_m^{(0)}$ and integrating over the space variables,

$$\int \sum_{m} \psi_{m}^{(0)*} a_{n}^{(1)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} d^{3}r = \int \psi_{m}^{(0)*} (E_{1} - H') \psi_{m}^{(0)} d^{3}r$$

Using the orthonormality of $\psi_n^{(0)}$,

$$\int \psi_m^{(0)} \ \psi_n^{(0)} \, d^3r = 0 \quad \text{if } m \neq n$$
=1 if $m = n$;

we have from the above equation that,

$$0 = \int \psi_m^{(0)*} (E_1 - H') \psi_m^{(0)} d^3r$$

Since E_1 is first order energy correction, it can be taken outside the integration treating as constant,

$$E_{1} = \int \psi_{m}^{(0)} \psi_{m}^{(0)} d^{3}r = \int \psi_{m}^{(0)} H' \psi_{m}^{(0)} d^{3}r$$

$$E_{1} = \int \psi_{m}^{(0)} H' \psi_{m}^{(0)} r^{3}r$$

or

 $\left\{ \text{Using the normality of } \psi_m^{(0)} \right\}$

Denoting $\psi_m^{(0)}$ by the ket $|m\rangle$, we can write it in the bra and ket notations as:

$$E_1 = \langle m \mid H' \mid m \rangle \qquad ...(13)$$

Evaluation of First-order wave-function ψ_1 . In order to find out the wave-function we multiply equation (12) by $\psi_k^{(0)}$ and integrate it over all space, we get

$$\int \sum_{n} a_{n}^{(1)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{k}^{(0)*} \psi_{n}^{(0)} d^{3}r = \int \psi_{k}^{(0)*} (E_{1} - H') \psi_{m}^{(0)} d^{3}r$$

Using the orthonormality of the unperturbed functions $\psi_n^{(0)}$ we get

$$a_{k}^{(1)} (E_{k}^{(0)} - E_{m}^{(0)}) = -\int \psi_{k}^{(0)^{*}} H' \psi_{m}^{(0)} d^{3}r$$
or
$$a_{k}^{(1)} (E_{k}^{(0)} - E_{m}^{(0)}) = -\langle k \mid H' \mid m \rangle \Rightarrow a_{k}^{(1)} = \frac{-\langle k \mid H' \mid m \rangle}{(E_{k}^{(0)} - E_{m}^{(0)})}$$

or
$$a_n^{(1)} = \frac{-\langle n \mid H' \mid m \rangle}{E_n^{(0)} - E_m^{(0)}}$$
; $n \neq m$...(14)

Using eq. (14) into (10), we get the first order wave-function

$$\psi_{1} = \sum_{n}' \frac{\langle n | H' | m \rangle \psi_{n}^{(0)}}{E_{m}^{(0)} - E_{n}^{(0)}} \dots (15)$$

The prime on the summation indicates the omission of the term n=m in the summation, i.e., the summation is for $n\neq m$ only.

If we take $\lambda=1$ or include the parameter λ into H, then in the first order perturbation,

$$H = H^{(0)} + H'$$

$$E = E_0 + E_1 = E_m^{(0)} + \langle m \mid H' \mid m \rangle$$

and
$$\psi = \psi_0 + \psi_1 = \psi_m^{(0)} + \sum_{n \neq m} \frac{\langle n \mid H' \mid m \rangle \psi_n^{(0)}}{(E_m^{(0)} - E_n^{(0)})}$$

Evaluation of Second order energy E2. Using eqn. (8), we can write the second-order perturbation equation (7c) as:

$$(H^{(0)} - E_m^{(0)}) \psi_2 = (E_1 - H') \psi_1 + E_2 \psi_m^{(0)} \dots (16)$$

For the solution of this equation we expand ψ_1 and ψ_2 in terms of the complete set of unperturbed wave functions $\psi_n^{(0)}$:

$$\psi_1 = \sum_{n=1}^{\infty} a_n^{(1)} \psi_n^{(0)} \text{ and } \psi_2 = \sum_{n=1}^{\infty} a_n^{(2)} \psi_n^{(0)} \dots (17)$$

Substituting equations (17) into (16), we get

$$\sum_{n} a_{n}^{(2)} (H^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} = \sum_{n} a_{n}^{(1)} (E_{1} - H') \psi_{n}^{(0)} + E_{2} \psi_{m}^{(0)}$$
or
$$\sum_{n} a_{n}^{(2)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} = \sum_{n} a_{n}^{(1)} (E_{1} - H') \psi_{n}^{(0)} + E_{2} \psi_{m}^{(0)}$$
...(18)

Multiplying equation (18) by $\psi_m^{(0)*}$ and integrating space variables,

$$\int \psi_{m}^{(0)^{*}} \sum_{n} a_{n}^{(2)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} d^{3}r$$

$$= \int \psi_{m}^{(0)^{*}} \sum_{n} a_{n}^{(1)} (E_{1} - H') \psi_{n}^{(0)} d^{3}r + \int \psi_{m}^{(0)^{*}} E_{2} \psi_{m}^{(0)} d^{3}r$$
...(19)

For m=n, $(E_n^{(0)} - E_m^{(0)})$ vanishes and for $m \neq n$, $\int \psi_m^{(0)} \psi_n^{(0)} a^3 r$

vanishes; therefore, the integral on the left hand side of the above equation vanishes for all values of n. Also, for $n \neq m$, the first part of the first integral on the right hand side vanishes due to the orthonormality of $\psi_n^{(0)}$. Thus using the orthonormality of

functions $\psi_n^{(0)}$, we can write equation (19) as

or
$$0 = -\sum_{n \neq m} a_n^{(1)} \int \psi_m^{(0)} H' \psi_n^{(0)} d^3r + E_2$$

$$E_2 = \sum_{n} a_n^{(1)} \langle m \mid H' \mid n \rangle.$$

Substituting the value of $a_n^{(1)}$ from eqn. (14) into the above, we get

$$E_{2} = \sum_{n}^{\prime} \frac{\langle n \mid H' \mid m \rangle \langle m \mid H' \mid n \rangle}{(E_{m}^{(0)} - E_{n}^{(0)})} = \frac{2m}{...(20)}$$

As before, the prime on the summation indicates the omission of the term n=m.

Evaluation of Second-order Function ψ_2 . In order to evaluate the wave-function we multiply equation (18) by $\psi_k^{(0)}$ and integrate it over all space. we get

$$\int_{n}^{\infty} \psi_{k}^{(0)*} \sum_{n}^{\infty} a_{n}^{(2)} \left(E_{n}^{(0)} - E_{m}^{(0)} \right) \psi_{n}^{(0)} d^{3}r = \int_{n}^{\infty} \psi_{k}^{(0)*} \sum_{n}^{\infty} a_{n}^{(1)} \left(E_{1} - H' \right) \psi_{n}^{(0)} d^{3}r + \int_{n}^{\infty} \psi_{k}^{(0)*} E_{2} \psi_{n}^{(0)} d^{3}r.$$

Using the orthonormality of $\psi_n^{(0)}$'s we can write it as

$$a_k^{(2)} (E_k^{(0)} - E_m^{(0)}) = a_k^{(1)} E_1 - \sum_{n} a_n^{(1)} \langle k \mid H' \mid n \rangle.$$

Using eqns. (14) and (13) into it we write
$$a_k^{(2)} (E_k^{(0)} - E_m^{(0)}) = -\frac{\langle k \mid H' \mid m \rangle \langle m \mid H' \mid m \rangle}{(E_k^{(0)} - E_m^{(0)})}$$

$$+\sum_{n}' \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle}{(E_{n}^{(0)} - E_{m}^{(0)})}$$

or
$$a_k^{(2)} = \sum_{n=0}^{\infty} \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle - \langle k \mid H' \mid m \rangle \langle m \mid H' \mid m \rangle}{(E_m^{(0)} - E_n^{(0)}) (E_m^{(0)} - E_k^{(0)})} (E_m^{(0)} - E_k^{(0)})^3}$$
 $n \neq m. ...(21)$

Using eq. (21) into (17), we get the second-order wavefunction

$$\psi_{3} = \sum_{k} a_{k}^{(2)} \psi_{k}^{(0)} = \sum_{k} \psi_{k}^{(0)} \left[\sum_{n} \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle}{\langle E_{m}^{(0)} - E_{m}^{(0)} \rangle} (E_{m}^{(0)} - E_{k}^{(0)}) \right]$$

$$- \frac{\langle k \mid H' \mid m \rangle \langle m \mid H' \mid m \rangle}{\langle E_{m}^{(0)} - E_{k}^{(0)} \rangle^{2}}(22)$$

Hence the energy and the wavefunction for second order perturbation are given by

$$E = E_0 + E_1 + E_2 = E_m^{(0)} + \langle m \mid H' \mid m \rangle + \sum_{n}' \frac{|\langle m \mid H' \mid n \rangle|^2}{(E_m^{(0)} - E_n^{(0)})}$$

and
$$\psi = \psi_0 + \psi_1 + \psi_2$$

$$= \psi_m^{(0)} + \sum_{k}' \psi_k^{(0)} \left[\frac{\langle k \mid H' \mid m \rangle}{\langle E_m^{(0)} - E_k^{(0)} \rangle} \left(1 - \frac{\langle m \mid H' \mid m \rangle}{\langle E_m^{(0)} - E_k^{(0)} \rangle} \right) + \sum_{n}' \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle}{\langle E_m^{(0)} - E_k^{(0)} \rangle} \right],$$

where the primes over summations denote the omission of the terms k=m or n=m, as the case may be.

8.3. TIME-INDEPENDENT RERTURBATION THEORY FOR DEGENERATE CASE:

The non-degenerate perturbation method is not applicable when the energy level of the unperturbed system is degenerate. This is due to the fact that in the non-degenerate perturbation theory it was assumed that the perturbed wavefunction differs slightly from one function $\psi_m^{(0)}$, which is the solution of the unperturbed wave equation for a given energy value, whereas in case

of degenerate level there are several such functions which correspond to the same energy. For simplicity we first consider the case of a doubly degenerate level. Let $\psi_m^{(0)} \& \psi_l^{(0)}$ be two orthonormal eigenfunctions belonging to the level $E_m^{(0)}$. Since $\psi_m^{(0)}$ and $\psi_l^{(0)}$ are states corresponding to unperturbed energy; therefore, their linear combination will also be a state corresponding to this energy. Hence we write,

$$\psi_0 = a_m \psi_m^{(0)} + a_i \psi_i^{(0)}. \tag{23}$$

Substituting this value into the first order perturbation equaiton (7b), we get

$$(H^{(0}-E_0)\psi_1=(E_1-H')(a_m\psi_m^{(0)}+a_l\psi_l^{(0)}). \qquad ...(24)$$

Multiplying eq. (24) by $\psi_m^{(0)}$ and integrating over the entire space, we get

$$\int \psi_{m}^{(0)*} (H^{(0)} - E_{0}) \psi_{1} d^{3}r = \int \psi_{m}^{(0)*} (E_{1} - H') a_{m} \psi_{m}^{(0)} d^{3}r$$

$$+ \int \psi_{m}^{(0)*} (E_{1} - H') a_{i} \psi_{i}^{(0)} d^{3}r. \dots (25)$$

We have,

$$\int \psi_m^{(0)*} H^{(0)} \psi_1 d^3r = \int [H^{(0)} \psi_m^{(0)}]^* \psi_1 d^3r \ \{ :: H^{(0)} \text{ is Hermitian} \}$$

$$= \int [E_m^{(0)} \psi_m^{(0)}]^* \psi_1 d^3r$$

$$= E_m^{(0)} \int \psi_m^{(0)*} \psi_1 d^3r \ \{ :: E_m^{(0)} \text{ is real} \}(26)$$

Also $E_0 = E_m^{(0)}$. Therefore, using eq. (26) we see that the left hand side of eq. (25) vanishes. Hence equation (25) gives

$$\int \phi_m^{(0)^*} (E_1 - H') \ a_m \psi_m^{(0)} \ d^3r + \int \psi_m^{(0)*} (E_1 - H') \ a_l \ \psi_l^{(0)} \ d^3r = 0$$

$$\dots (27)$$
or $a_m E_1 \int \psi_m^{(0)*} \psi_m^{(0)} \ d^3r - a_m \int \psi_m^{(0)*} \ H' \psi_m^{(0)} \ d^3r + a_l E_1 \int \phi_m^{(0)*} \ \psi_l^{(0)} \ d^3r$

$$- a_l \int \psi_m^{(0)*} H' \psi_l^{(0)} \ d^3r = 0. \dots (28)$$

Using the orthonormality of $\psi_m^{(0)}$ and $\psi_l^{(0)}$, this equation reduces to

$$a_m E_1 - a_m \langle m \mid H' \mid m \rangle - a_l \langle m \mid H' \mid l \rangle = 0$$
 ...(29)

or
$$(\langle m \mid H' \mid m) - E_1) a_m + \langle m \mid H' \mid l) a_l = 0$$

or $(H'_{mm} - E_1) a_m + H'_{ml} a_l = 0.$...(30)

Similarly, multiplying eq. (24) by $\psi_{\ell}^{(0)*}$ and integrating over the entire space, we get

$$H'_{lm} a_m + (H'_{ll} - E_1) a_l = 0.$$
 ...(31)

Equations (30) and (31) are two homogeneous equations for a_m and a_l and they have a non-zero solution only if the determinant of coefficients, *i.e.*

$$H'_{lm} - E_1$$
 $H'_{ml} = 0.$

This is called the secular equation for the problem. It is a second degree algebraic equation for E_1 . Explicitly,

$$E_{1}^{2}-(H'_{mm}+H'_{ll})E_{1}+(H'_{mm}H'_{ll}-H'_{ml}H'_{lm})=0;$$

$$E_{1}=\frac{1}{2}\left[H'_{mm}+H'_{ll}\right]\pm\frac{1}{2}\left[\{H'_{mm}-H'_{ll}\}^{2}+4H'_{ml}H'_{lm}\right]^{1/2}. ...(32)$$

Thus, there are two possible values of E_1 , say $E_1^{(1)}$ and $E_1^{(2)}$. For Hermitian operator H', both of these values are real. Hence the original energy level splits into two levels, $E_m^{(0)} + E_1^{(1)}$ and $E_m^{(0)} + E_2^{(2)}$, as a result of the perturbation. We say that the perturbation removes the degeneracy. It may happen however that for some perturbations $E_1^{(1)} = E_1^{(2)}$, in such cases the degeneracy would still remain and in order to remove the degeneracy we have to go for higher-order perturbation calculations.

Removal of Degeneracy in Second order Perturbation. Using eq. (23) into the second-order perturbation equation (7c), we get:

$$(H^{(0)}-E_0) \psi_2 = (E_1-H') \psi_1 + E_2 (a_m \psi_m^{(0)} + a_l \psi_l^{(0)}). \qquad ...(33)$$

Taking its scalar product with $\psi_m^{(0)}$, we see that the left hand side vanishes as in the first order perturbation and hence,

$$\int \psi_m^{(0)*} (E_1 - H') \psi_1 d^3r + \int \psi_m^{(0)*} E_2 (a_m \psi_m^{(0)} + a_i \psi_i^{(0)}) d^3r = 0.$$

a very good approximation for the solution of Schrodinger equation at time t' is obtained by assuming the instantaneous value, H(t'), of Hamiltonian as constant. The stationary state wavefunctions at time t' satisfy the equation

$$H(t') \psi_n(\mathbf{r}, t') = E_n(t') \psi_n(\mathbf{r}, t')$$
 ...(72)

Now, we expand the soln. of eqn. (71), ψ , in terms of functions ψ_n in the following way

$$\psi = \sum_{n} a_n(t) \ \psi_n \ \exp. \left[-\frac{i}{\hbar} \int_0^t E_n(t') \ dt' \right] \qquad \dots (73)$$

where we assume that ψ_n 's are orthonormal, discrete and nondegenerate. Using this ψ into eqn. (71) we get

$$i\hbar \sum_{n} \left(\dot{a}_{n}\psi_{n} + a_{n} \frac{\partial \psi_{n}}{\partial t} \right) \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right]$$

$$+ \sum_{n} a_{n}\psi_{n}E_{n} \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right]$$

$$= \sum_{n} \left(a_{n}E_{n}\psi_{n} \right) \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right]$$

$$\{ :: H\psi_{n} = E_{n}\psi_{n} \}$$

$$\{ :: H\psi_{n} = E_{n}\psi_{n} \}$$

or
$$\sum_{n} \left(\dot{a}_{n} \psi_{n} + a_{n} \frac{\partial \psi_{n}}{\partial i} \right) \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right] = 0 \qquad ...(74)$$

Multiplying eqn. (74) by

$$\psi_m^* \exp \left[\frac{i}{\hbar} \int_0^t E_m(t') dt'\right]$$

and integrating over all space, we obtain

$$\int \sum_{n} d_{n} \psi_{m}^{*} \psi_{n} \exp \left[\frac{i}{\hbar} \int_{0}^{t} E_{m}(t') dt' - \frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt'\right] d^{3}r$$

$$+ \sum_{n} a_{n} \int \psi_{m}^{*} \frac{\partial \psi_{n}}{\partial t} \exp \left[\frac{i}{\hbar} \int_{0}^{t} E_{m}(t') dt' - \frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt'\right] d^{3}r = 0$$

Using orthonormality of ψ_n 's we have

$$a_m = -\sum_{m=0}^{\infty} a_m \int \psi_m^* \frac{\partial \psi_n}{\partial t} \exp \left[-\frac{i}{\hbar} \int_0^t (E_n - E_m) dt' \right] d^3r$$

In the development of quantum mechanics, only a few simple physical problems like Hydrogen atom, harmonic oscillator and rigid rotator etc. could be solved completely and exactly. However in practice, exactly solvable problems are rare, i.e., for the majority of systems of physical interest, the exact solution of the Schroedinger equation presents great mathematical difficulties. In order to permit the discussion of these systems, various methods of approximate solutions of the wave equation have been devised, leading to more or less accurate approximate evaluation of energy values and wave-functions. Really speaking, there are as many approximation methods as there are problems and there is no question of treating them all here. In this book we present only three most general methods which are useful under different conditions.

8.1. PERTURBATION METHODS:

Out of these methods, a simple and beautiful one is wave mechanical perturbation theory daveloped by Schroedinger in 1926. If the problem at hand is sufficiently similar to one that has an exact solution, the Hamiltonian can be broken up into two parts, one of which is large and characterizes the system for which the Schroedinger equation can be solved exactly, while the other part is small and can be treated as a perturbation. Perturbation theories are of two kinds:

- (i) time-independent perturbation theory and
- (ii) time-dependent perturbation theory.

In the time-independent method, Hamiltonian does not depend on time, while in the time-dependent method Hamiltonian depends explicitly on time.

TIME-INDEPENDENT PERTURBATION THEORY FOR NON-DEGENERATE CASE:

Let us suppose that the discrete set of all the eigenvalues $E_{-}^{(0)}$ and the orthonormal set of eigenfunctions $\psi_n^{(0)}$ of the unperturbed Hamiltonian H(0) of a system are known,

$$H^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}, \dots (1)$$

in which $E_n^{(0)}$ is the energy of the nth level of the system with the corresponding state function as $\psi_n^{(0)}$. Now, if a small perturbation is added to the system so that the Hamiltonian changes to H, then the energy levels and the stationary states of the system are given by the solution of the eigenvalue equation

 $H\psi = E\psi$ Usulally this equation is not exactly soluble. The perturbation theory provides a systematic method of successive approximations to the eigenfunction ψ and the eigenvalue E in terms of the unperturbed eigenfunctions $\psi_n^{(0)}$ and eigenvalues $E_n^{(0)}$. The basic idea is to split up H into the unperturbed Hamiltonian $H^{(0)}$ plus a perturbation part H',

 $H=H^{(0)}+\lambda H'$

where the small parameter λ characterizes the strength of the perturbation*.

We now develop the perturbation theory assuming that E and ψ can be expressed as power series in λ such that the zero, the first. etc, powers of λ correspond to the zero, the first etc. orders of approximation,

$$\psi = \psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \dots
E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots$$
(4)

Substituting Eqs. (4) and (5) in Eq. (2) and grouping the terms of the same order together, we have

$$\frac{e^2}{c\hbar} \approx \frac{1}{137}$$

^{*}For example, when the unperturbed system is an atom, and the perturbation is due to electromagnetic field acting on it, the parameter λ is the fine

$$(H^{(0)}-E_0) \psi_0 + [(H^{(0)}-E_0) \psi_1 + (H'-E_1) \psi_0] \lambda + [(H^{(0)}-E_0) \psi_2 + (H'-E_1) \psi_1 - E_2 \psi_0] \lambda^2 + \dots = 0 \qquad \dots (6)$$

We want this equation to be valid for any arbitrary (but small) strength of the perturbation, i.e., for any value of λ . This can happen only if the co-efficient of each power of λ vanishes. Thus we should have

$$(H^{(0)}-E_0)\psi_0=0$$
 ...(7a)

$$(H^{(0)}-E_0) \psi_1=(E_1-H') \psi_0$$
 ...(7b)

$$(H^{(0)}-E_0) \psi_2=(E_1-H') \psi_1+E_2 \psi_0$$
 ...(7c)

etc. These are the zeroth order, first order, second order, ..., equations of the perturbation theory. The zeroth order equation (7a) means that ψ_0 is any one of the unperturbed eigenfunctions. Let us take

$$\psi_0 = \psi_m^{(0)}$$
 and $E_0 = E_m^{(0)}$...(8)

and suppose that $\psi_m^{(0)}$ is non-degenerate.

Evaluation of first-order energy E₁. Using eq. (8), we can write the first-order perturbation equation (7b) as:

$$(H^{(0)}-E_m^{(0)}) \psi_1=(E_1-H') \psi_m^{(0)}$$
 ...(9)

For the solution of this equation we expand ψ_1 in terms of the complete set of unperturbed wave functions $\psi_n^{(0)}$,

$$\psi_1 = \sum_{n=1}^{\infty} a_n^{(1)} \psi_n^{(0)} \dots (10)$$

$$H^{(0)}\psi_1 = \sum_{n} a_n^{(1)} H^{(0)} \psi_n^{(0)}$$

$$= \sum_{n}^{\infty} a_n^{(1)} E_n^{(0)} \psi_n^{(0)} \dots (11)$$

Substituting equations (10) and (11) into (9). we have

$$\sum_{n} a_{n}^{(1)} E_{n}^{(0)} \psi_{m}^{(0)} - E_{m}^{(0)} \sum_{n} a_{n}^{(1)} \psi_{n}^{(0)} = (E_{1} - H') \psi_{m}^{(0)}$$

or
$$\sum_{n} a_n^{(1)} (E_n^{(0)} - E_m^{(0)}) \psi_n^{(0)} = (E_1 - H') \psi_m^{(0)}$$
 ...(12)

Multiplying equation (12) by $\psi_m^{(0)}^*$ and integrating over the space variables,

$$\int \sum_{m} \psi_{m}^{(0)*} a_{n}^{(1)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} d^{3}r = \int \psi_{m}^{(0)*} (E_{1} - H') \psi_{m}^{(0)} d^{3}r$$

Using the orthonormality of $\psi_n^{(0)}$,

$$\int \psi_m^{(0)} \ \psi_n^{(0)} \, d^3r = 0 \quad \text{if } m \neq n$$
=1 if $m = n$;

we have from the above equation that,

$$0 = \int \psi_m^{(0)*} (E_1 - H') \psi_m^{(0)} d^3r$$

Since E_1 is first order energy correction, it can be taken outside the integration treating as constant,

$$E_{1} = \int \psi_{m}^{(0)} \psi_{m}^{(0)} d^{3}r = \int \psi_{m}^{(0)} H' \psi_{m}^{(0)} d^{3}r$$

$$E_{1} = \int \psi_{m}^{(0)} H' \psi_{m}^{(0)} r^{3}r$$

or

 $\left\{ \text{Using the normality of } \psi_m^{(0)} \right\}$

Denoting $\psi_m^{(0)}$ by the ket $|m\rangle$, we can write it in the bra and ket notations as:

$$E_1 = \langle m \mid H' \mid m \rangle \qquad ...(13)$$

Evaluation of First-order wave-function ψ_1 . In order to find out the wave-function we multiply equation (12) by $\psi_k^{(0)*}$ and integrate it over all space, we get

$$\int \sum_{n} a_{n}^{(1)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{k}^{(0)*} \psi_{n}^{(0)} d^{3}r = \int \psi_{k}^{(0)*} (E_{1} - H') \psi_{m}^{(0)} d^{3}r$$

Using the orthonormality of the unperturbed functions $\psi_n^{(0)}$ we get

$$a_{k}^{(1)} (E_{k}^{(0)} - E_{m}^{(0)}) = -\int \psi_{k}^{(0)^{*}} H' \psi_{m}^{(0)} d^{3}r$$
or
$$a_{k}^{(1)} (E_{k}^{(0)} - E_{m}^{(0)}) = -\langle k \mid H' \mid m \rangle \Rightarrow a_{k}^{(1)} = \frac{-\langle k \mid H' \mid m \rangle}{(E_{k}^{(0)} - E_{m}^{(0)})}$$

or
$$a_n^{(1)} = \frac{-\langle n \mid H' \mid m \rangle}{E_n^{(0)} - E_m^{(0)}}$$
; $n \neq m$...(14)

Using eq. (14) into (10), we get the first order wave-function

$$\psi_{1} = \sum_{n}' \frac{\langle n | H' | m \rangle \psi_{n}^{(0)}}{E_{m}^{(0)} - E_{n}^{(0)}} \dots (15)$$

The prime on the summation indicates the omission of the term n=m in the summation, i.e., the summation is for $n\neq m$ only.

If we take $\lambda=1$ or include the parameter λ into H, then in the first order perturbation,

$$H = H^{(0)} + H'$$

$$E = E_0 + E_1 = E_m^{(0)} + \langle m \mid H' \mid m \rangle$$

and
$$\psi = \psi_0 + \psi_1 = \psi_m^{(0)} + \sum_{n \neq m} \frac{\langle n \mid H' \mid m \rangle \psi_n^{(0)}}{(E_m^{(0)} - E_n^{(0)})}$$

Evaluation of Second order energy E2. Using eqn. (8), we can write the second-order perturbation equation (7c) as:

$$(H^{(0)} - E_m^{(0)}) \psi_2 = (E_1 - H') \psi_1 + E_2 \psi_m^{(0)} \dots (16)$$

For the solution of this equation we expand ψ_1 and ψ_2 in terms of the complete set of unperturbed wave functions $\psi_n^{(0)}$:

$$\psi_1 = \sum_{n=1}^{\infty} a_n^{(1)} \psi_n^{(0)} \text{ and } \psi_2 = \sum_{n=1}^{\infty} a_n^{(2)} \psi_n^{(0)} \dots (17)$$

Substituting equations (17) into (16), we get

$$\sum_{n} a_{n}^{(2)} (H^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} = \sum_{n} a_{n}^{(1)} (E_{1} - H') \psi_{n}^{(0)} + E_{2} \psi_{m}^{(0)}$$
or
$$\sum_{n} a_{n}^{(2)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} = \sum_{n} a_{n}^{(1)} (E_{1} - H') \psi_{n}^{(0)} + E_{2} \psi_{m}^{(0)}$$
...(18)

Multiplying equation (18) by $\psi_m^{(0)*}$ and integrating space variables,

$$\int \psi_{m}^{(0)^{*}} \sum_{n} a_{n}^{(2)} (E_{n}^{(0)} - E_{m}^{(0)}) \psi_{n}^{(0)} d^{3}r$$

$$= \int \psi_{m}^{(0)^{*}} \sum_{n} a_{n}^{(1)} (E_{1} - H') \psi_{n}^{(0)} d^{3}r + \int \psi_{m}^{(0)^{*}} E_{2} \psi_{m}^{(0)} d^{3}r$$
...(19)

For m=n, $(E_n^{(0)} - E_m^{(0)})$ vanishes and for $m \neq n$, $\int \psi_m^{(0)} \psi_n^{(0)} a^3 r$

vanishes; therefore, the integral on the left hand side of the above equation vanishes for all values of n. Also, for $n \neq m$, the first part of the first integral on the right hand side vanishes due to the orthonormality of $\psi_n^{(0)}$. Thus using the orthonormality of

functions $\psi_n^{(0)}$, we can write equation (19) as

or
$$0 = -\sum_{n \neq m} a_n^{(1)} \int \psi_m^{(0)} H' \psi_n^{(0)} d^3r + E_2$$

$$E_2 = \sum_{n} a_n^{(1)} \langle m \mid H' \mid n \rangle.$$

Substituting the value of $a_n^{(1)}$ from eqn. (14) into the above, we get

$$E_{2} = \sum_{n}^{\prime} \frac{\langle n \mid H' \mid m \rangle \langle m \mid H' \mid n \rangle}{(E_{m}^{(0)} - E_{n}^{(0)})} = \frac{2m}{...(20)}$$

As before, the prime on the summation indicates the omission of the term n=m.

Evaluation of Second-order Function ψ_2 . In order to evaluate the wave-function we multiply equation (18) by $\psi_k^{(0)}$ and integrate it over all space. we get

$$\int_{n}^{\infty} \psi_{k}^{(0)*} \sum_{n}^{\infty} a_{n}^{(2)} \left(E_{n}^{(0)} - E_{m}^{(0)} \right) \psi_{n}^{(0)} d^{3}r = \int_{n}^{\infty} \psi_{k}^{(0)*} \sum_{n}^{\infty} a_{n}^{(1)} \left(E_{1} - H' \right) \psi_{n}^{(0)} d^{3}r + \int_{n}^{\infty} \psi_{k}^{(0)*} E_{2} \psi_{n}^{(0)} d^{3}r.$$

Using the orthonormality of $\psi_n^{(0)}$'s we can write it as

$$a_k^{(2)} (E_k^{(0)} - E_m^{(0)}) = a_k^{(1)} E_1 - \sum_{n} a_n^{(1)} \langle k \mid H' \mid n \rangle.$$

Using eqns. (14) and (13) into it we write
$$a_k^{(2)} (E_k^{(0)} - E_m^{(0)}) = -\frac{\langle k \mid H' \mid m \rangle \langle m \mid H' \mid m \rangle}{(E_k^{(0)} - E_m^{(0)})}$$

$$+\sum_{n}' \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle}{(E_{n}^{(0)} - E_{m}^{(0)})}$$

or
$$a_k^{(2)} = \sum_{n=0}^{\infty} \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle - \langle k \mid H' \mid m \rangle \langle m \mid H' \mid m \rangle}{(E_m^{(0)} - E_n^{(0)}) (E_m^{(0)} - E_k^{(0)})} (E_m^{(0)} - E_k^{(0)})^3}$$
 $n \neq m. ...(21)$

Using eq. (21) into (17), we get the second-order wavefunction

$$\psi_{3} = \sum_{k} a_{k}^{(2)} \psi_{k}^{(0)} = \sum_{k} \psi_{k}^{(0)} \left[\sum_{n} \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle}{\langle E_{m}^{(0)} - E_{m}^{(0)} \rangle} (E_{m}^{(0)} - E_{k}^{(0)}) \right]$$

$$- \frac{\langle k \mid H' \mid m \rangle \langle m \mid H' \mid m \rangle}{\langle E_{m}^{(0)} - E_{k}^{(0)} \rangle^{2}}(22)$$

Hence the energy and the wavefunction for second order perturbation are given by

$$E = E_0 + E_1 + E_2 = E_m^{(0)} + \langle m \mid H' \mid m \rangle + \sum_{n}' \frac{|\langle m \mid H' \mid n \rangle|^2}{(E_m^{(0)} - E_n^{(0)})}$$

and
$$\psi = \psi_0 + \psi_1 + \psi_2$$

$$= \psi_m^{(0)} + \sum_{k}' \psi_k^{(0)} \left[\frac{\langle k \mid H' \mid m \rangle}{\langle E_m^{(0)} - E_k^{(0)} \rangle} \left(1 - \frac{\langle m \mid H' \mid m \rangle}{\langle E_m^{(0)} - E_k^{(0)} \rangle} \right) + \sum_{n}' \frac{\langle k \mid H' \mid n \rangle \langle n \mid H' \mid m \rangle}{\langle E_m^{(0)} - E_k^{(0)} \rangle} \right],$$

where the primes over summations denote the omission of the terms k=m or n=m, as the case may be.

8.3. TIME-INDEPENDENT RERTURBATION THEORY FOR DEGENERATE CASE:

The non-degenerate perturbation method is not applicable when the energy level of the unperturbed system is degenerate. This is due to the fact that in the non-degenerate perturbation theory it was assumed that the perturbed wavefunction differs slightly from one function $\psi_m^{(0)}$, which is the solution of the unperturbed wave equation for a given energy value, whereas in case

of degenerate level there are several such functions which correspond to the same energy. For simplicity we first consider the case of a doubly degenerate level. Let $\psi_m^{(0)} \& \psi_l^{(0)}$ be two orthonormal eigenfunctions belonging to the level $E_m^{(0)}$. Since $\psi_m^{(0)}$ and $\psi_l^{(0)}$ are states corresponding to unperturbed energy; therefore, their linear combination will also be a state corresponding to this energy. Hence we write,

$$\psi_0 = a_m \psi_m^{(0)} + a_i \psi_i^{(0)}. \tag{23}$$

Substituting this value into the first order perturbation equaiton (7b), we get

$$(H^{(0}-E_0)\psi_1=(E_1-H')(a_m\psi_m^{(0)}+a_l\psi_l^{(0)}). \qquad ...(24)$$

Multiplying eq. (24) by $\psi_m^{(0)}$ and integrating over the entire space, we get

$$\int \psi_{m}^{(0)*} (H^{(0)} - E_{0}) \psi_{1} d^{3}r = \int \psi_{m}^{(0)*} (E_{1} - H') a_{m} \psi_{m}^{(0)} d^{3}r$$

$$+ \int \psi_{m}^{(0)*} (E_{1} - H') a_{i} \psi_{i}^{(0)} d^{3}r. \dots (25)$$

We have,

$$\int \psi_m^{(0)*} H^{(0)} \psi_1 d^3r = \int [H^{(0)} \psi_m^{(0)}]^* \psi_1 d^3r \ \{ :: H^{(0)} \text{ is Hermitian} \}$$

$$= \int [E_m^{(0)} \psi_m^{(0)}]^* \psi_1 d^3r$$

$$= E_m^{(0)} \int \psi_m^{(0)*} \psi_1 d^3r \ \{ :: E_m^{(0)} \text{ is real} \}(26)$$

Also $E_0 = E_m^{(0)}$. Therefore, using eq. (26) we see that the left hand side of eq. (25) vanishes. Hence equation (25) gives

$$\int \phi_m^{(0)^*} (E_1 - H') \ a_m \psi_m^{(0)} \ d^3r + \int \psi_m^{(0)*} (E_1 - H') \ a_l \ \psi_l^{(0)} \ d^3r = 0$$

$$\dots (27)$$
or $a_m E_1 \int \psi_m^{(0)*} \psi_m^{(0)} \ d^3r - a_m \int \psi_m^{(0)*} \ H' \psi_m^{(0)} \ d^3r + a_l E_1 \int \phi_m^{(0)*} \ \psi_l^{(0)} \ d^3r$

$$- a_l \int \psi_m^{(0)*} H' \psi_l^{(0)} \ d^3r = 0. \dots (28)$$

Using the orthonormality of $\psi_m^{(0)}$ and $\psi_l^{(0)}$, this equation reduces to

$$a_m E_1 - a_m \langle m \mid H' \mid m \rangle - a_l \langle m \mid H' \mid l \rangle = 0$$
 ...(29)

or
$$(\langle m \mid H' \mid m) - E_1) a_m + \langle m \mid H' \mid l) a_l = 0$$

or $(H'_{mm} - E_1) a_m + H'_{ml} a_l = 0.$...(30)

Similarly, multiplying eq. (24) by $\psi_{\ell}^{(0)*}$ and integrating over the entire space, we get

$$H'_{lm} a_m + (H'_{ll} - E_1) a_l = 0.$$
 ...(31)

Equations (30) and (31) are two homogeneous equations for a_m and a_l and they have a non-zero solution only if the determinant of coefficients, *i.e.*

$$H'_{lm} - E_1$$
 $H'_{ml} = 0.$

This is called the secular equation for the problem. It is a second degree algebraic equation for E_1 . Explicitly,

$$E_{1}^{2}-(H'_{mm}+H'_{ll})E_{1}+(H'_{mm}H'_{ll}-H'_{ml}H'_{lm})=0;$$

$$E_{1}=\frac{1}{2}\left[H'_{mm}+H'_{ll}\right]\pm\frac{1}{2}\left[\{H'_{mm}-H'_{ll}\}^{2}+4H'_{ml}H'_{lm}\right]^{1/2}. ...(32)$$

Thus, there are two possible values of E_1 , say $E_1^{(1)}$ and $E_1^{(2)}$. For Hermitian operator H', both of these values are real. Hence the original energy level splits into two levels, $E_m^{(0)} + E_1^{(1)}$ and $E_m^{(0)} + E_2^{(2)}$, as a result of the perturbation. We say that the perturbation removes the degeneracy. It may happen however that for some perturbations $E_1^{(1)} = E_1^{(2)}$, in such cases the degeneracy would still remain and in order to remove the degeneracy we have to go for higher-order perturbation calculations.

Removal of Degeneracy in Second order Perturbation. Using eq. (23) into the second-order perturbation equation (7c), we get:

$$(H^{(0)}-E_0) \psi_2 = (E_1-H') \psi_1 + E_2 (a_m \psi_m^{(0)} + a_l \psi_l^{(0)}). \qquad ...(33)$$

Taking its scalar product with $\psi_m^{(0)}$, we see that the left hand side vanishes as in the first order perturbation and hence,

$$\int \psi_m^{(0)*} (E_1 - H') \psi_1 d^3r + \int \psi_m^{(0)*} E_2 (a_m \psi_m^{(0)} + a_i \psi_i^{(0)}) d^3r = 0.$$

Using
$$\psi_1 = \sum_{n} a_n^{(1)} \psi_n^{(0)}$$
, $\int \psi_m^{(0)} \psi_n^* \psi_1 d^3r = 0$ and
$$\int \psi_m^{(0)} \psi_l^{(0)} d^3r = 0 \text{ for } m \neq l,$$

we can write eqn. (34) as

$$-\int \psi_m^{(0)*} H' \sum_n a_n^{(1)} \psi_n^{(0)} d^3r + a_m E_2 \int \psi_m^{(0)*} \psi_m^{(0)} d^3r = 0 \text{ for } m \neq l$$

$$\sum_{n=0}^{\infty} a_n^{(1)} \int a_n^{(1)} d^3r + a_m E_2 \int a_n^{(0)*} \psi_m^{(0)} d^3r = 0 \text{ for } m \neq l$$

or $\sum_{n=0}^{\infty} a_n^{(1)} H'_{mn} - a_m E_2 = 0. \qquad ...(35)$

Similarly, multiplying eq. (33) by $\psi_i^{(0)*}$ and integrating over the entire space, we get

$$\sum_{n} a_{n}^{(1)} H'_{1n} - a_{1}E_{2} = 0. \qquad(36)$$

Now to find the value of $a_n^{(1)}$, we multiply equation (24) by $\psi_k^{(0)*}$ and integrate it over the space variables; we get

$$\int \psi_{k}^{(0)*} \sum_{n} (H^{(0)} - E_{0}) \ a_{n}^{(1)} \ \psi_{n}^{(0)} \ d^{3}r$$

$$= \int \psi_{k}^{(0)*} (E_{1} - H') \ (a_{m} \psi_{m}^{(0)} + a_{l} \psi_{l}^{(0)}) \ d^{3}r$$
or
$$\sum_{n} a_{n}^{(1)} (E_{n}^{(0)} - E_{m}^{(0)}) \int \psi_{k}^{(0)*} \psi_{n}^{(0)} \ d^{3}r$$

$$= a_{m} E_{1} \int \psi_{k}^{(0)*} \psi_{m}^{(0)} \ d^{3}r + a_{l} E_{1} \int \psi_{k}^{(0)*} \psi_{l}^{(0)} \ d^{3}r$$

$$- a_{m} \int \psi_{k}^{(0)*} H' \psi_{m}^{(0)} \ d^{3}r - a_{l} \int \psi_{k}^{(0)*} H' \psi_{l}^{(0)} \ d^{3}r$$

or $a_k^{(1)}(E_k^{(0)}-E_m^{(0)})=-a_mH'_{km}-a_lH'_{kl}$

{using the orthonormality of $\psi_n^{(0)}$'s}

$$\Rightarrow a_k^{(1)} = \frac{a_m H'_{km} + a_l H'_{kl}}{E_m^{(0)} - E_k^{(0)}}; m \neq k$$

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$$a_n^{(1)} = \frac{a_m H'_{nm} + a_l H'_{nl}}{E_m^{(0)} - E_n^{(0)}}; m \neq n, \qquad ...(37)$$

Using eq, (37) into (35) and 36, we obtain

$$\sum_{n \neq l, m} \frac{a_m H'_{nm} + a_l H'_{nl}}{E_m^{(0)} - E_n^{(0)}} H'_{mn} - E_2 a_m = 0, \dots (38)$$

$$\sum_{n \neq l, m} \frac{a_m H'_{nm} + a_l H'_{nl}}{E_m^{(0)} - E_n^{(0)}} H'_{ln} - E_2 a_l = 0. \quad ...(39)$$

The secular equation associated with these equations gives solutions for E_2 which are of the same general form as that for E_1 . These roots are equal if

$$\sum_{n \neq l, m} \frac{H'_{mn}H'_{nm}}{E_m^{(0)} - E_n^{(0)}} = \sum_{n \neq l, m} \frac{H'_{ln}H'_{nl}}{E_m^{(0)} - E_n^{(0)}}$$
and
$$\sum_{n \neq l, m} \frac{H'_{mn}H'_{nl}}{E_m^{(0)} - E_n^{(0)}} = 0.$$

and

Unless both of these equations are satisfied, the degeneracy is removed in second order perturbation,

α-Fold degenerate case. Generalization of the above treatment to the case of α -fold degeneracy is straightforward. Let $\psi_m^{(0)}$, $\psi_m^{(0)}$,

....., $\psi_{m\alpha}^{(0)}$ be α orthonormal eigenfunctions belonging to the

level $E_m^{(0)}$. Since all these states are the eigenfunction for the unperturbed energy, their linear combination will also be a state Hence we write corresponding to this energy,

$$\psi_0 = \sum_{n=1}^{\alpha} a_n \, \psi_{mn}^{(0)} \qquad \dots (41)$$

Substituting this value into the first drder perturbation equation, (7b), we get:

$$\left(H^{(0)} - E_m^{(0)} \right) \psi_1 = (E_1 - H') \sum_{n=1}^{\alpha} a_n \psi_{m \cdot n}^{(0)} \qquad \dots (42)$$

Multiplying eq. (42) by $\psi_{m_1}^{(0)*}$ and intergrating over the entre space we get:

$$\int \psi_{m_1}^{(0)*} \left(H^{(0)} - H_m^{(0)} \right) \psi_1 d^3 r = E_1 a_1 \int \psi_{m_1}^{(0)*} \psi_{m_1}^{(0)} dr^3$$

$$+ E_1 \sum_{n=2}^{\alpha} a_n \int \psi_{m_1}^{(0)*} \psi_{mn}^{(0)} d^3 r - \sum_{n=1}^{\alpha} a_n \int \psi_{m_1}^{(0)*} H' \psi_{mn}^{(0)} d^3 r. \dots (43)$$

The feft hand side of above equation is zero as in the case of double degeneracy. Now using the orthonormality of $\psi_{mn}^{(0)}$'s and the notations

$$\int \psi_{m_1}^{(0)*} H' \psi_{mn}^{(0)} d^3r = H'_{1n} \qquad \dots (44)$$

we can write eq. (43) as,

or

$$0 = E_1 a_1 - a_1 H'_{11} - a_2 H'_{12} - a_3 H'_{13} \dots - a_{\alpha} H'_{1\alpha}$$

$$(H'_{11} - E_1) a_1 + H'_{12} a_2 + \dots + H'_{1\alpha} a_{\alpha} = 0 \qquad \dots (45a)$$

Similarly, multiplying eq. (42) by $\psi_{m_2}^{(0)*}$, $\psi_{m_3}^{(0)*}$,..., $\psi_{m\alpha}^{(0)*}$ and integrating over the space, we get:

$$H'_{21}a_1 + (H'_{22} - E_1) \ a_2 + \dots + H'_{2n}a_n = 0 \qquad \dots (45b)$$
...

$$H'_{\alpha_1}a_1 + H'_{\alpha_2}a_2 + \dots + (H'_{\alpha\alpha} - E_1) a_{\alpha} = 0$$
 ...(45\alpha)

Eqns. (45) are homogeneous equations for $a_1, ..., a_{\alpha} a_2$, and they have a nonzero solution only if the determinant coefficients vanishes ie.,

This is the secular equation for the problem. On evaluating the determinant, equation (46) is a polynomial of degree α in E_1 , and has α roots $E_{1\mu}$ ($\mu=1, 2, ..., \alpha$). Hence the original energy level $E_m^{(0)}$ splits (in general) into an α -plet, $\left(E_m^{(0)} + E_{1\mu}\right)$ ($\mu=1, 2, ..., \alpha$), i.e., the perturbation removes the degeneracy.

8.8. TIME-DEPENDENT PERTURBATION THEORY:

So far we have assumed the Hamiltonian operator H to be independent of time. When the Hamiltonian has a small part which depends on the time, the above time-independent perturbation theory is not applicable. The theory of time dependent perturbation was developed by Dirac and is often called as the

theory of the variation of constants. As in time-independent perturbation theory, we assume that

$$H^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)} \dots (47)$$

However, the small perturbation H' now depends on the time and has the effect of causing transitions between eigenstates of $H^{(0)}$, which are stationary in the absence of H'. Since the Hamiltonian, $H=H^{(0)}+H'$, depends on time, we must now work with the time-dependent Schroedinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = (H^{(0)} + H')\psi \qquad(48)$$

A general solution of eq. (48) can be written in terms of the eigenfunctions $\psi_n^{(0)} \exp \left[-iE_n^{(0)} t/\hbar\right]$ see equation (90), chapter-1 of the unperturbed time-dependent equation as follows

$$\psi = \sum_{n} a_{n}(t) \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\}, \quad ...(49)$$

 $\left\{ :: H_n^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)} \right\}.$

where the expansion coefficients evidently depend on time.

Substituting eq. (49) into (48) we get:

$$i\hbar \frac{\partial}{\partial t} \left[\sum_{n} a_{n}(t) \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\} \right]$$

$$= (H^{(0)} + H') \left[\sum_{n} a_{n}(t) \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\} \right]$$
or
$$\sum_{n} i\hbar \frac{\partial}{\partial t} \left[\int_{n} a_{n}(t) \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\} \right]$$

$$+ \sum_{n} a_{n}(t) E_{n}^{(0)} \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\}$$

$$= \sum_{n} a_{n}(t) E_{n}^{(0)} \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\}$$

$$+ \sum_{n} a_{n}(t) H' \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\}$$

"APPROXIMATE METHODS FOR BOUND STATE PROBLEMS"

Cancelling the common terms on both sides, we get

Cancelling the contains
$$\sum_{n} i\hbar \, \tilde{a}_{n}(t) \, \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\}$$

$$= \sum_{n} a_{n}(t) \, H' \, \psi_{n}^{(0)} \exp \left\{ -iE_{n}^{(0)} t/\hbar \right\} \quad ...(50)$$

Multiplying both sides of eq. (50) by $\psi_k^{(0)}$ and integrating

over the space, we get

over the space,
$$\sum_{n} i\hbar \dot{a}_{n}(t) \exp. \left\{ -iE_{n}^{(0)} t/\hbar \right\} \int \psi_{k}^{(0)*} \psi_{n}^{(0)} d^{3}r$$

$$= \sum_{n} a_{n}(t) \exp. \left\{ -iE_{n}^{(0)}t/\hbar \right\} \int \psi_{k}^{(0)*} H' \psi_{n}^{(0)} d^{3}r.$$
or
$$\sum_{n} i\hbar \dot{a}_{n}(t) \exp. \left\{ -iE_{n}^{(0)} t/\hbar \right\} \delta_{kn}$$

$$= \sum_{n} a_{n}(t) \exp. \left\{ -iE_{n}^{(0)} t/\hbar \right\} H'_{kn}$$

 $\left\{ \text{ From orthonormality of functions } \psi_n^{(0)} \right\}$

or $i\hbar \dot{a}_k(t) \exp\left\{-iE_k^{(0)}t/\hbar\right\} = \sum_n a_n(t) \exp\left\{-iE_n^{(0)}t/\hbar\right\} H'_{kn}$

or
$$\dot{a}_k(t) = (i\hbar)^{-1} \sum_{n} H'_{kn} a_n(t) \exp\{i\omega_{kn}t\}$$
 ...(51)

where we have,

$$\omega_{kn} = \frac{E_k^{(0)} - E_n^{(0)}}{\hbar}, \qquad ...(52)$$

known as Bohr's or Angular frequency.

Equation (51) is an infinite set of simultaneous differential equations in the function $a_k(t)$. These can be solved for some particular cases as shown below:

Let us suppose that when the perturbation is applied at t=0, all except one of the a_n are zero, so that the system is in a definite unperturbed energy state. We thus take

$$a_n(t) = 0$$
 for $n \neq k$
= 1 for $n = k$; at $t = 0$
 $a_n(t) = \delta_{nk}$ at $t = 0$

Thus, we can find the solution of equation (51) numerically, but physically it cannot be done, since there are infinite number of equations.

If the small perturbation H' acts on the system for a short time, it can be treated as independent of time during this period. Hence we may solve equation (51) by neglecting all terms on the right hand side except that with n=k, that is, by assuming that only the term in $a_k(t)$ needs be retained on the right side of these equation. Thus

$$\dot{a}_k(t) = (i\hbar)^{-1} a_k(t) H'_{kk}$$

s we get. ...(54)

Integrating this we get,

$$a_k(t) = \exp\left[-\frac{1}{i\hbar} \cdot H'_{kk} t\right] \qquad \dots (55)$$

The constant of integration is zero due to the assumption that $a_k(0)=1$.

The equation (55) tells us the way in which the coefficient $a_k(t)$ changes during the time when the perturbation is acting.

Now let us consider the remaining of the equations (51) which determine 'the behaviour of the coefficients $a_k(t)$ with $k \neq n$. Replacing $a_n(t)$ on the right hand side of equation (51) by its initial value $a_n(0) = 1$ and neglecting all other a_n 's we obtain

$$\dot{a}_k(t) = (i\hbar)^{-1} H'_{kn} e^{i\omega_{kn}t}$$
 ...(56)

Let the field be switched on at t=0 and switched off at t=t. During this period the perturbation, H' remains constant; and before and after the application of field it is zero. On integrating equation (56), we get

$$a_{k}(t) = (i\hbar)^{-1} H'_{kn} \int_{0}^{t} e^{i\omega_{kn}t'} dt'$$

$$= (i\hbar)^{-1} H'_{kn} \frac{e^{i\omega_{kn}t} - 1}{i\omega_{kn}} = -H'_{kn} \frac{e^{i\omega_{kn}t} - 1}{\hbar\omega_{kn}} \qquad ...(57)$$
effore the real difference of the state
Therefore, the probability of finding the system in kth state at any time t can be calculated as follows:

Probability=
$$|a_{k}(t)|^{2}=|H'_{kn}|^{2}\frac{(e^{i\omega_{kn}t}-1)(e^{-i\omega_{kn}t}-1)}{\hbar^{2}\omega^{2}_{kn}}$$

= $|H'_{kn}|^{2}\frac{2-2\cos\omega_{kn}t}{\hbar^{2}\omega^{2}_{kn}}$

or
$$|a_k(t)|^2 = \frac{4|H'_{kn}|^2 \sin^2(\omega_{kn}t/2)}{\hbar^2 \omega_{kn}^2}$$
 ...(58)

The factor $\sin^2(\omega_{kn}t/2)/\omega_{kn}^2$ is plotted as a function of ω_{kn} in figure 1.

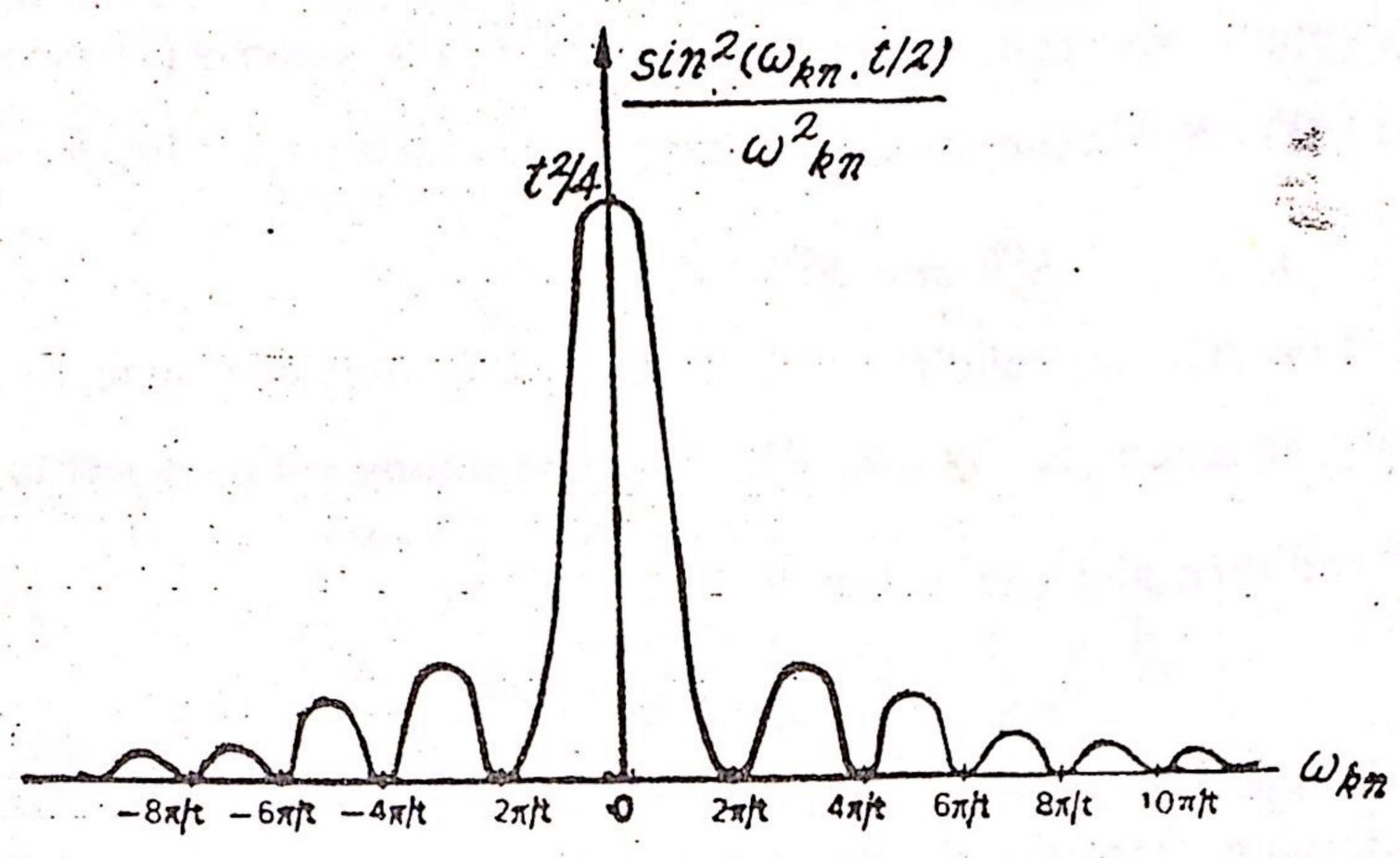


Fig. 1.

Taking $\omega_{kn} = x$, we write

$$\frac{\sin^2(xt/2)}{x^2} = \frac{1}{x^2} \left[\left(\frac{xt}{2} \right) - \frac{(xt)^3}{3 \cdot 2} + \dots \right]^2$$

The maximum value of $\frac{\sin^2(xt/2)}{x^2}$ occurs when x=0. Therefore,

$$\left[\frac{\sin^2(xt/2)}{x^2}\right]_{max} = \frac{\text{Lim}}{x \to 0} \left[\frac{\sin^2(xt/2)}{x^2}\right] = \frac{t^2}{4} \qquad ...(59)$$

Hence the peak value of $\sin^2(\omega_{kn}t/2)/\omega_{kn}^2$ is $t^2/4$ as shown in in the graph.

The value of $\frac{\sin^2(xt/2)}{x^2}$ will be zero when

$$\sin (xt/2) = 0 \text{ or } \frac{xt}{2} = \pm n\pi \text{ or } x = \pm \frac{2n\pi}{t}.$$

$$\therefore \omega_{kn} = \pm \frac{2\pi n}{t} \qquad \dots (60)$$

It is quite clear from figure 1 that the height of the main peak increases in proportion to t^2 while its breadth decreases inversely as t. Therefore the area under the curve is prorpotional to t. Thus, if there is a group of states that have energies nearly equal to the initial state, the probability of finding the system in one or another of these states is proportional to t. This statement

implies that the probability per unit time that a transition has taken place when the perturbation has been on for a time t is proportional to t.

If the final states form a continum, as in the case of ionization of an atom, we can define the density of final states P(k) such that P(k) $dE_k^{(0)}$ is the number of final states with energies between

$$E_k^{(0)}$$
 and $E_k^{(0)} + dE_k^{(0)}$

Transition probability per unit time. It is obtained by multiplying equation (58) by $\rho(k) dE_k^{(0)}$ and integrating with respect to $E_k^{(0)}$ and then dividing by time t, i.e.,

$$w = \frac{1}{t} \int |a_k(t)|^2 P(k) dE_k^{(0)} \dots (61)$$

If the central peak is the domain of integration (i.e. energy conserving transitions), the main contribution comes from this peak and only small error is involved in extending the limit of this integral to $-\infty$ to $+\infty$.

$$w = \frac{1}{t} \int_{-\infty}^{+\infty} \frac{4|H'_{kn}|^2 \sin^2(\omega_{kn} t/2)}{\hbar^2 \omega_{kn}^2} \rho(k) dE_k^{(0)} \dots (62)$$

As t becomes large, then according to fig. 1 breadth of the main peak becomes small. We can regard quantities H'_{kn} and $\rho(k)$ sufficiently independent of $E_k^{(0)}$ and hence they can be taken outside the integral. Therefore,

$$w = \frac{2\hbar |H'_{kn}|^2 \rho(k)}{\hbar^2} \int_{-\infty}^{+\infty} \frac{\sin^2(\omega_{kn}t/2)}{(\omega_{kn}t/2)^2} d(\omega_{kn}t/2)$$

$$\left[: dE_k^{(0)} = \hbar \omega_{kn} \text{ as } E_k^{(0)} - E_n^{(0)} = \hbar \omega_{kn} \right]$$

or putting $\frac{\omega_{kn}t}{2} = x$

$$w = \frac{2\hbar |H'_{kn}|^2 \rho(k)}{\hbar^2} \int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx$$

$$= \frac{2\hbar |H'_{kn}|^2 \rho(k)}{\hbar^2} .\pi$$

$$w = \frac{2\pi}{\hbar} P(k) |H'_{kn}|^2$$

..(63)

This formula has got wide applications in quantum physics.

Harmonic Perturbation. If the perturbation H' depends harmonically on the time except for being turned on at time t=0 and turned off at a later time $t=t_0$, we can write

$$H'_{kn} = \begin{cases} 2 (H'_0)_{kn} \sin \omega t \text{ for } 0 < t < t_0 \\ 0 & \text{elsewhere} \end{cases} \dots (64)$$

where $(H'_0)_{kn}$ is independent of time and $\omega > 0$. Then the integration of eqn. (56) gives:

$$a_k(t) = \frac{2 (H'_0)_{kn}}{i\hbar} \int_0^t \sin \omega t' \exp \{i\omega_{kn}t'\} dt' \text{ for } t < t_0 \qquad ...(65)$$

and
$$a_k(t) = \frac{2(H'_0)_{kn}}{i\hbar} \int_0^{t_0} \sin \omega t' \exp \{i\omega_{kn}t'\} dt' \text{ for } t \ge t_0$$

we get

$$a_{k} (t \geqslant t_{0}) = \frac{-(H'_{0})_{kn}}{i\hbar} \left[\frac{\exp \left[i \left\{\omega_{kn} + \omega\right\} t_{0}\right] - 1}{\omega_{kn} + \omega} - \frac{\exp \left[i \left\{\omega_{kn} - \omega\right\} t_{0}\right] - 1}{\omega_{kn} - \omega} \right] \dots (66)$$

From eqn. (66) it is apparant that the amplitude is appreciable only when the denominator of one or the other of the two terms is practically zero. If the denominator of first term is zero, then

or
$$E_{k}^{(0)} - E_{n}^{(0)}$$

$$E_{k}^{(0)} - h\omega$$

$$E_{k}^{(0)} = E_{n}^{(0)} - h\omega \qquad ...(67a)$$

Similarly, the denominator of second term gives,

$$E_k^{(0)} = E_n^{(0)} + \hbar \omega$$
 ...(67b)

From eqns. (67a) and (67b) we see that the first term is important when the effect of the perturbation is to transfer to the system on which it acts the Planck's quantum of energy $\hbar \omega$. If the effect of the perturbation is to receive from the system the quantum of energy $\hbar \omega$, the second term will be important. Now if we assume that the initial state n is a discrete bound state and the final state

k is one of a continuous set of dissociated states, then $E_k^{(0)} > E_n^{(0)}$, and only the second term in (66) needs be considered, i.e.

$$a_k (t \ge t_0) = \frac{(H'_0)_{km}}{i\hbar} \cdot \frac{e^{i(\omega_{kn} - \omega)} t_0}{\omega_{kn} - \omega}$$

Hence the probability of finding the system in kth state after the perturbation is removed is:

$$|a_k(t \ge t_0)|^2 = \frac{4 |(H'_0)_{kn}|^2 \sin^2[(\omega_{kn} - \omega) t_0/2]}{\hbar^2 (\omega_{kn} - \omega)^2} \dots (68)$$

This is identical to equation (58) for the constant perturbation with the only difference that the role of ω_{kn} is played by $(\omega_{kn}-\omega)$ here. A graph between $\sin^2[(\omega_{kn}-\omega) t_0/2]/(\omega_{kn}-\omega)^2$ and $(\omega_{kn}-\omega)$ is identical to that of figure 1. The height of the main peak is $t_0^2/4$ and its breadth decreases inversely as t_0 , so that the area under the curve is proportional to t_0 . Similar to the constant perturbation, the transition probability per unit time to a group of states k that have energies nearly equal to $E_n^{(0)} + \hbar \omega$, is given by

$$w = \frac{1}{t_0} \int |a_k(t \ge t_0)|^2 \rho(k) dE_k^{(0)} \qquad ...(69)$$

where $\rho(k) dE_k^{(0)}$ is the number of final states with energies bet-

ween $E_k^{(0)}$ and $E_k^{(0)} + dE_k^{(0)}$, $\rho(k)$ is energy density of final state.

As t_0 becomes large, the breadth of the main peak becomes small. We can regard $(H'_0)_{km}$ and P(k) as quantities sufficiently independent of $E_k^{(0)}$ and can take them outside the integral. Therefore substitution of eqn. (68) into eqn. (69) gives

$$w = \frac{2\pi}{\hbar} \rho(k) | (H'_0)_{kn}|^2 \qquad ...(70)$$

8.5. ADIABATIC PERTURBATION:

Time dependent perturbation theory is used to solve the problems for which the Hamiltonian has a small part which depends on time. We now extend this theory to solve more general problems in which the perturbation part undergoes large changes.

Now we wish to solve the Schroedinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H(t) \psi \qquad ...(71)$$

when H(t) varies slowly with time. If H(t) varies slowly enough,

a very good approximation for the solution of Schrodinger equation at time t' is obtained by assuming the instantaneous value, H(t'), of Hamiltonian as constant. The stationary state wavefunctions at time t' satisfy the equation

$$H(t') \psi_n(\mathbf{r}, t') = E_n(t') \psi_n(\mathbf{r}, t')$$
 ...(72)

Now, we expand the soln. of eqn. (71), ψ , in terms of functions ψ_n in the following way

$$\psi = \sum_{n} a_n(t) \ \psi_n \ \exp. \left[-\frac{i}{\hbar} \int_0^t E_n(t') \ dt' \right] \qquad \dots (73)$$

where we assume that ψ_n 's are orthonormal, discrete and nondegenerate. Using this ψ into eqn. (71) we get

$$i\hbar \sum_{n} \left(\dot{a}_{n}\psi_{n} + a_{n} \frac{\partial \psi_{n}}{\partial t} \right) \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right]$$

$$+ \sum_{n} a_{n}\psi_{n}E_{n} \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right]$$

$$= \sum_{n} \left(a_{n}E_{n}\psi_{n} \right) \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right]$$

$$\{ :: H\psi_{n} = E_{n}\psi_{n} \}$$

$$\{ :: H\psi_{n} = E_{n}\psi_{n} \}$$

or
$$\sum_{n} \left(\dot{a}_{n} \psi_{n} + a_{n} \frac{\partial \psi_{n}}{\partial i} \right) \exp \left[-\frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt' \right] = 0 \qquad ...(74)$$

Multiplying eqn. (74) by

$$\psi_m^* \exp \left[\frac{i}{\hbar} \int_0^t E_m(t') dt'\right]$$

and integrating over all space, we obtain

$$\int \sum_{n} d_{n} \psi_{m}^{*} \psi_{n} \exp \left[\frac{i}{\hbar} \int_{0}^{t} E_{m}(t') dt' - \frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt'\right] d^{3}r$$

$$+ \sum_{n} a_{n} \int \psi_{m}^{*} \frac{\partial \psi_{n}}{\partial t} \exp \left[\frac{i}{\hbar} \int_{0}^{t} E_{m}(t') dt' - \frac{i}{\hbar} \int_{0}^{t} E_{n}(t') dt'\right] d^{3}r = 0$$

Using orthonormality of ψ_n 's we have

$$a_m = -\sum_{m=0}^{\infty} a_m \int \psi_m^* \frac{\partial \psi_n}{\partial t} \exp \left[-\frac{i}{\hbar} \int_0^t (E_n - E_m) dt' \right] d^3r$$

$$= -\sum_{n} a_{n} \exp \left[-\frac{i}{\hbar} \int_{0}^{t} (E_{n} - E_{m}) dt' \int \psi_{m}^{*} \frac{\partial \psi_{n}}{\partial t} d^{3}r \right] \dots (75)$$

To evaluate the integral in this equation, differentiating equation (72) we obtain

$$\frac{\partial H}{\partial t} \psi_n + H \frac{\partial \psi_n}{\partial t} = \frac{\partial E_n}{\partial t} \psi_n + E_n \frac{\partial \psi_n}{\partial t} ...$$

Multiplying it by ψ_m^* ($m \neq n$) and integrating over the space, we get:

$$\int \psi_m^* \frac{\partial H}{\partial t} \psi_n d^3r + \int \psi_m^* H \frac{\partial \psi_n}{\partial t} d^3r = \frac{\partial E_n}{\partial t} \int \psi_m^* \psi_n d^3r + E_n \int \psi_m^* \frac{\partial \psi_n}{\partial t} d^3r$$

Using the fact that H is hermitian and the orthonormality of ψ_n 's this eqn. can be written as

$$\int \psi_{m}^{*} \frac{\partial H}{\partial t} \psi_{n} d^{3}r + \int (H\psi_{m})^{*} \frac{\partial \psi_{n}}{\partial t} d^{3}r = E_{n} \int \psi_{m}^{*} \frac{\partial \psi_{n}}{\partial t} d^{3}r$$
or
$$\int \psi_{m}^{*} \frac{\partial H}{\partial t} \psi_{n} d^{3}r + E_{m} \int \psi_{m}^{*} \frac{\partial \psi_{n}}{\partial t} d^{3}r = E_{n} \int \psi_{m}^{*} \frac{\partial \psi_{n}}{\partial t} d^{3}r$$
or
$$(E_{m} - E_{n}) \langle \psi_{m} | \dot{\psi}_{n} \rangle = - \langle \psi_{m} | \frac{\partial H}{\partial t} | \psi_{n} \rangle; m \neq n \dots (76)$$

Substituting (76) into 75 we get:

$$\dot{a}_{m} = \sum_{n \neq m} \frac{a_{n} \int \psi_{m}^{*} \frac{\partial H}{\partial t} \psi_{n} d^{3}r}{(E_{m} - E_{n})} \text{ exp.} \left[-\frac{i}{\hbar} \int_{0}^{t} (E_{n} - E_{m}) dt' \right], \text{ or}$$

$$\dot{a}_{m} = \sum_{n \neq m} \frac{a_{n}}{\hbar \omega_{mn}} \left\langle m \left| \frac{\partial H}{\partial t} \right| n \right\rangle \text{ exp.} \left[i \int_{0}^{t} \omega_{mn}(t') dt' \right] \dots (77)$$

Let us suppose that the system is in a definite unperturbed energy state at t=0, so that we can put $a_n=\delta_{nk}$. We thus obtain

$$\dot{a}_m \simeq (\hbar \omega_{mk})^{-1} \left\langle m \left| \frac{\partial H}{\partial t} \right| k \right\rangle \exp \left[i \int_0^t \omega_{mk}(t') dt' \right]; k \neq m$$
...(78)

We can now evaluate a_m by assuming that all the quantities $\left(\omega_{mk}, \psi_n \text{ and } \frac{\partial H}{\partial t}\right)$

appearing on the right hand side of eqn. (78), which are expected to be slowly varying, are constant in time and can be taken outside the integral. Therefore we obtain

$$a_{m} \simeq (\hbar \omega_{mk})^{-1} \left\langle m \left| \frac{\partial H}{\partial t} \right| k \right\rangle \int_{0}^{t} \exp \left[i \omega_{mk} t' \, dt' \right]; \, k \neq m$$

$$= (i \hbar \omega_{mk}^{2})^{-1} \left\langle m \left| \frac{\partial H}{\partial t} \right| k \right\rangle \left[\exp \left(i \omega_{mk} t \right) - 1 \right]; \, k \neq m \quad ...(79)$$

According to equation (79), the amplitude for states other than the initial state oscillates in time and do not show any steady increase over long periods of time even if H changes by an appreciable amount. Thus a negligible error is made by neglecting the probability, $|a_m|^2$, of finding the system in the final state ψ_m and in saying that the system remains in the initial state ψ_k even though ψ_k itself is changing with time. This is known as adiabatic approximation. A very good example of adiabatic approximation is met in the Molecular Physics, where the motion of the nuclei (due to their large mass) is much smaller than that of the electrons around them. Therefore it is a good approximation to take the nuclei as fixed for calculating the electronic motion. Moreover, the nuclear motion can be calculated under the assumption that the electrons have their steady motion for each instantaneous arrangement of the nuclei (adiabatic approximation.

An Example of Adiabatic Approximation. As a simple example of the application of adiabatic approximation, we consider a linear harmonic oscillator for which the position, a(t), of the equilibrium point depends on time. Hamiltonian for this oscillator is given by

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} K \left[x - a(t) \right]^2 \qquad ...(80)$$

The instantaneous energy eigenfunctions are the harmonic-oscillator wavefunctions centered at the point a(t), and the energy levels are unchanged.

$$\psi_n(x) = N_n H_n[\alpha(x-a)] \exp[-\frac{1}{2}\alpha^2(x-a)^2]; E_n = (n+\frac{1}{2})\hbar\omega$$
 ...(81) where,

$$\alpha^4 = \frac{mK}{\hbar^2}$$

If the oscillator is initially in its ground state (n=0), the time derivative of the hamiltonian, $\frac{\partial H}{\partial t} = -K(x-a)\dot{a}$, has a nonvanishing matrix element only with the first excited state. This can be evaluated using;

$$\int \psi_n^* x \, \psi_m \, dx = \begin{cases} \frac{1}{\alpha} \left(\frac{n+1}{2}\right)^{1/2} & m = n+1\\ \frac{1}{\alpha} \left(\frac{n}{2}\right)^{1/2} & m = n-1\\ 0 & \text{otherwise.} \end{cases} \dots (82)$$

We get, $\langle 1 | \frac{\partial H}{\partial t} | 0 \rangle = -\frac{K\dot{a}}{\alpha \sqrt{(2)}} = -K\dot{a} \left(\frac{\hbar}{2}\right)^{1/2} (mK)^{-1/4} ...(83)$

Substituting this into eqn. (79) we get the magnitude of the coefficient of the time dependent factor in the amplitude of the first excited state, as

$$\frac{K\dot{a}}{\hbar\omega^2} \cdot \frac{(\hbar/2)^{1/2}}{(Km)^{1/4}} = \frac{\dot{a}}{(2\hbar\omega/m)^{1/2}}...(84)$$

Equation (84) may be interpreted physically by noting that the denominator is of the order of the maximum speed of a hypothetical classical oscillator with the zero point energy. Thus the adiabatic approximation is good when the equilibrium point moves slowly in comparison with the classical oscillator speed.

8.6. SUDDEN APPROXIMATION:

The sudden approximation is used when the change in the Hamiltonian occupies a very short but finite interval of time. For this, let us suppose that at time t=0, the Hamiltonian suddenly changes from H_0 to H_1 and remains constant thereafter, i.e.,

$$H = \begin{cases} H_0 \text{ for } t < 0 \\ H_1 \text{ for } t > 0 \end{cases} \dots (85)$$

Then the wavefunctions are given by,

$$H_0 \ \psi_n^{(0)} = E_n^{(0)} \ \psi_n^{(0)} \text{ for } t < 0$$

$$H_1 \ \psi_m^{(1)} = E_m^{(1)} \ \psi_m^{(1)} \text{ for } t > 0 \qquad \dots (86)$$

where $\psi_n^{(0)}$'s and $\psi_m^{(1)}$'s form complete orthonormal sets of functions.

Therefore the general solution can be written as:

$$\psi = \begin{cases} \sum_{n}^{\infty} a_n \, \psi_n^{(0)} \, \exp(-iE_n^{(0)} t/\hbar) & \text{for } t < 0 \\ \sum_{m}^{\infty} b_m \, \psi_m^{(1)} \, \exp(-iE_m^{(1)} t/\hbar) & t \text{ for } > 0 \end{cases} \dots (87)$$

Since the wave equation $i\hbar \frac{\partial \psi}{\partial t} = H\psi$ is of first order in the

time, the wavefunction at each point in space must be a continuous function of time. The condition of continuity at t=0 gives

$$\sum_{n} a_n \psi_n^{(0)} = \sum_{m} b_m \psi_m^{(1)}$$

Multiplying the above equation by $\psi_m^{(1)*}$ and integrating over the entire space we get:

$$b_{m} = \sum_{n} a_{n} \int \psi_{m}^{(1)*} \psi_{n}^{(0)} d^{3}r$$

$$b_{m} = \sum_{n} a_{n} \langle m \mid n \rangle \qquad ...(88)$$

or

According to sudden approximation we can use the above equation (88) even when the change in the Hamiltonian takes a very short but finite interval of time t_0 . We suppose

$$H = \begin{cases} H_0 \text{ for } t < 0 \\ H_i \text{ for } 0 < t < t_0 \\ H_1 \text{ for } t > t_0 \end{cases} \dots (89)$$

The intermediate Hamiltonian, which is assumed to be constant in time, has a complete set of energy eigenfunctions, given by

$$H_i \psi_k^{(i)} = E_k^{(i)} \psi_k^{(i)}$$
 ...(90)

The exact solution can be expanded in terms of $\psi_k^{(i)}$'s with constant co-efficients

$$\psi = \sum_{k} C_k \psi_k^{(i)} \exp. (-iE_k^{(i)} t/\hbar) \text{ for } 0 < t < t_0$$
 ...(91)

Applying continuity condition at t=0 we get

$$C_k = \sum_{n} a_n \langle k \mid n \rangle \qquad \dots (92)$$

Similarly, the continuity condition at $t=t_0$ gives

$$b_m = \sum_k C_k \langle m \mid k \rangle \exp \left[-i \left(E_k^{(i)} - E_m^{(1)} \right) t_0 / \hbar \right]$$

$$= \sum_{n} a_{n} \sum_{k} \langle m \mid k \rangle \langle k \mid n \rangle \exp \left[-i \left(E_{k}^{(i)} - E_{m}^{(1)}\right) t_{0}/\hbar\right] \dots (93)$$

For $t_0 = 0$, the exponential is equal to unity and eqn. (93) reduces to eqn. (88) as it should be.

For sudden approximation to be good, t_0 should be very small. Then we can expand the exponential term in eqn. (93) as follows

$$b_{m} \simeq \sum_{n} a_{n} \sum_{k} \langle m \mid k \rangle \left\{ 1 - \frac{it_{0}}{\hbar} \left(E_{k}^{(i)} - E_{m}^{(1)} \right) \right\} \langle k \mid n \rangle$$

$$= \sum_{n} a_{n} \langle m \mid \left\{ 1 - \frac{it_{0}}{\hbar} \left(H_{i} - H_{1} \right) \mid n \right\} \qquad \dots (94)$$

Comparing it with eqn. (88) we see that the error in the sudden approximation is proportional to t_0 for small t_0 , and it can be estimated from eqn. (94).

8.7. THE VARIATIONAL METHOD

The perturbation, theory applicable to those problems for which the Hamiltonian differs only slightly from the Hamiltonian $H^{(0)}$, for which the Schroedinger equation can be solved exactly. Now we describe a method, known as the variational method, which is applicable even when there is no closely related problem that can be solved exactly. This method is primarily used for the estimation of the ground state energy of a system. It can also be applied to the systems that are described by a non-separable Schroedinger equation. Variational method is based upon the following principle:

The expectation value of the Hamiltonian in any state ψ of a system is never smaller than the energy of E_0 of the ground state of the system. To show this, we expand ψ in terms of the orthonormal set of eigen-functions ψ_k of H as

$$\psi = \sum a_k \ \psi_k, H \ \psi_k = E_k \psi_k, \int \psi_k^* \ \psi_l \ d^3r = \delta_{kl} \qquad \dots (95)$$

Now expectation value of H for the function ψ is given by

$$\langle H \rangle = \int \psi^* H \psi \ d^3r = \int \sum_{k} a_k^* \psi_k^* H \sum_{l} a_l \ \psi_l \ d^3r = \sum_{k, l} a_k^* a_l \ E_l \ \delta_{kl}$$
$$= \sum_{k} |a_k|^2 E_k \qquad ... (96)$$

On replacing each of the eigenvalues E_k in eqn. (96) by the lowest eigenvalue E_0 , we obtain the inequality,

$$\langle H \rangle \geqslant \sum_{k} |a_{k}|^{2} E_{0} = E_{0} \sum_{k} |a_{k}|^{2} = E_{0} \dots (97)$$

We have made use of the fact $\sum_{k} |a_k|^2 = 1$ for a normalized wavefunction ψ .

If ψ differs from the eigenfunction ψ_0 of the ground state by a small quantity of the order of ϵ , then $\langle H \rangle$ with differ from E_0 by a small quantity of the order of ϵ^2 . To prove this, let us take

$$\psi = \psi_0 + \epsilon \phi \qquad ...(98)$$

Then,

$$\langle H \rangle = \int (\psi_0 + \epsilon \, \phi)^* \, H \, (\psi_0 + \epsilon \, \phi) \, d^3r$$

$$= \int \psi_0^* \, H \, \psi_0 \, d^3r + \epsilon \int \psi_0^* \, H \, \phi \, d^3r + \epsilon \int \phi^* \, H \, \psi_0 \, d^3r$$

$$+\epsilon^{2} \int \phi^{*} H \phi d^{3}r.$$

$$=E_{0} \int \psi_{0}^{*} \psi_{0} d^{3}r + \epsilon E_{0} \int \psi_{0}^{*} \phi d^{3}r + \epsilon E_{0} \int \phi^{*} \psi_{0} d^{3}r$$

$$+\epsilon^{2} \int \phi^{*} H \phi d^{3}r \quad \{ : H \text{ is hermitian} \}$$

$$=E_{0} + \epsilon^{2} E^{(2)} : \text{ where, } E^{(2)} = \int \phi^{*} H \phi d^{3}r \qquad \dots (99)$$

$$\{ : \psi_{0} \text{ and } \phi \text{ are orthogonal to each other} \}$$

Equation (97) shows that smaller the value of $\langle H \rangle$, the closer it will be to E_0 . Therefore, the variational method consists in minimizing $\langle H \rangle$ by varying ψ and taking the minimum value of $\langle II \rangle$ as an estimate for E_0 . In practice, we always have some information about the general form of the wavefunction, and most of the times it is possible to write a trial wave function in terms of suitably chosen function containing one or more parameters; on the basis of physical intuition. Equation (97) can then be used to compute $\langle H \rangle$ as a function of these parameters, and the parameters can be adjusted to minimize $\langle H \rangle$. This minimum value of $\langle H \rangle$ is the best estimate of E_0 , obtainable with a wavefunction of the chosen form. Because of the second order nature of the approximation, the value of $\langle H \rangle$ is, in general, a much better approximation to E_0 than the corresponding ψ to the ground-state wavefunction ψ_0 .

The variational method can also be used to calculate an upper limit for one of the higher energy levels. If we choose a trial wave function ψ which is orthogonal to the wave functions ψ_0 , ψ_1 , ..., ψ_{m-1} ; then the coefficients a_0 , a_1 , ..., a_{m-1} in the expansion (96) obviously vanish and the lowest energy which appears in the expression $\Sigma \mid a_k \mid^2 E_k$ will be E_m . We then obtain

$$\langle H \rangle \geqslant E_m$$
 ...(100)

Thus the expectation value of H gives an upper bound for the mth energy level E_m .

Trial Function Linear in Variational Parameters. In many problems, especially in molecular physics, trial wave functions are chosen as linear combinations of known functions, as

$$\psi = c_1 u_1 + c_2 u_2 + \ldots + c_r u_r, \qquad \ldots (101)$$

with the coefficients $c_1, c_2, ..., c_r$ as variational parameters. The u_i 's are not necessarily orthonormal to each other. Then,

$$\langle H \rangle = \sum_{i, j=1}^{r} C_i^* C_j H_{ij}$$
, where $H_{ij} = \int u_i^* H u_j d^3r$...(102)

We have to minimize $\langle H \rangle$ w.r.t. the C_i subject to the constriant that ψ be normalized i.e.

$$\int \psi^* \psi \ d^3r = \sum c_i^* c_j \triangle_{ij} = 1, \text{ where } \triangle_{ij} = \int u_i^* u_j \ d^3r \quad ...(103)$$

We use the method of Lagrange multiplier to take into account this constraint. Thus we require that the quantity

$$I = \sum c_i^* c_j H_{ij} - \lambda \left(\sum c_i^* c_j \triangle_{ij} - 1 \right) \qquad \dots (104)$$

be a minimum, where λ is the Lagrangian multiplier. For this, the derivative of I w.r.t. the real and the imaginary parts of c_i (or equivalently, with respect to c_i and c_i * treated as independent complex parameters) should be zero. From $\frac{\partial I}{\partial c_i} = 0$, we get

$$\sum_{j=1}^{r} (H_{ij} - \lambda \triangle_{ij}) \ a_j = 0, \ (i=1, 2, ..., r). \qquad ...(105)$$

The equations $\frac{\partial I}{\partial C_4} = 0$ are simply complex conjugates of

equations (105), and give nothing new. Equations (105) is a set of r homogeneous equations in r unknowns C_i . For a nontrivial solution of these equations, the determinant of the matrix of coefficients must vanish, i.e.

$$\begin{vmatrix} H_{11} - \lambda \triangle_{1l} & H_{12} - \lambda \triangle_{12} & \dots & H_{1r} - \lambda \triangle_{1r} \\ H_{21} - \lambda \triangle_{21} & H_{22} - \lambda \triangle_{22} & \dots & H_{2r} - \lambda \triangle_{2r} \\ \dots & \dots & \dots & \dots \\ H_{r_1} - \lambda \triangle_{r_1} & H_{r_2} - \lambda \triangle_{r_2} & \dots & H_{r_r} - \lambda \triangle_{r_r} \end{vmatrix} = 0. \quad \dots (106)$$

This is an algebraic equation of degree r in λ and have r roots $\lambda_1, \lambda_2, ..., \lambda_r$. These are the possible values of $\langle H \rangle$, because

$$\langle H \rangle = \sum_{ij} H_{ij} C_i^* C_j = \lambda \sum_{ij} \sum_{ij} C_i^* C_j = \lambda$$
 ...(107)
 ij {Using eqns. (102), (105) and (103)}

Minimum of the values $\lambda_1, \lambda_2, ..., \lambda_r$, provides the best estimate of the ground state energy E_0 .

8.8. THE WKB APPROXIMATION:

The WKB approximation stands for the Wentzel-Kramer-Brillouin approximation and it leads to the Bohr-Sommerfeld quantization rules of old quantum theory from the Schroedinger

equation. It is, therefore, a semi-classical approximation and it is based on the expansion of the wavefunction in powers of ħ, the first term of which leads to the classical results, the second term to the old quantum theory results and the higer terms are the characteristic of the new mechanics.

The one-dimensional Schroedinger equation,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left[E - V(x) \right] \psi = 0,$$

can be written in the form

$$\frac{d^2\psi}{dx^2} + k^2(x) \psi = 0, \qquad ...(108)$$

where k(x) is the propagation constant at the point x;

$$k(x) = \frac{\sqrt{2m[E-V(x)]}}{\hbar}$$
...(109)

The solution of eqn. (108) is of the form
$$\psi = A \exp \{i \ k(x) \ x\}. \tag{110}$$

For V(x) < E, we put it in the form

$$\psi = Ae^{iS(x)/\hbar}, \qquad \dots (111)$$

where S(x) is a function of x.

Substituting (111) into (108), we obtain
$$i\hbar S'' - S'^2 + \hbar^2 k^2 = 0.$$
 ...(112)

The WKB method obtains the first two terms (one term beyond the classical expression) of an expansion of S in powers of \hbar . We, therefore, substitute

$$S(x) = S_0 + \hbar S_1 + \dots$$
 ...(113)

into eqn. (112) We get

 $i\hbar \left[S_0'' + \hbar S_1'' + \hbar^2 S_2'' + \ldots\right] - \left[S_0' + \hbar S_1' + \hbar^2 S_2' + \ldots\right]^2 + \hbar^2 k^2 = 0$ or $i\hbar \left[S_0'' + \hbar S_1'' + \hbar^2 S_2'' + \ldots\right]$

$$-[S_0'^2 + 2\hbar S_0'S_1' + \hbar^2 (S_1'^2 + 2S_0'S_2') + \dots] + 2m [E - V(x)] = 0.$$
...(114)

Equating the coefficients of same powers of ħ on both sides of the above equation, we get

$$-S_0'^2 + 2m (E - V) = 0, \qquad ...(115a)$$

$$iS_0''-2S_0'S_1'=0,$$
 ...(115b)

$$iS_1'' - S_1'^2 - 2S_0'S_2' = 0$$
 etc. ...(115c)

From eqn. (115a). we have

$$\frac{dS_0}{dx} = \pm \sqrt{2m (E-V)} = \pm \hbar k (x)$$

$$S_0(x) = \pm \hbar \int_{x_0}^x k(x') dx'.$$
 ...(116)

From equation (115b), we have

$$\frac{dS_{1}}{dx} = \frac{i}{2} \frac{1}{(dS_{0}/dx)} \cdot \frac{d^{2}S_{0}}{dx^{2}}$$

$$= \frac{i}{2} \frac{d}{dx} \log \frac{dS_{0}}{dx}$$

$$\therefore S_{1} = \frac{i}{2} \log \frac{dS_{0}}{dx} = \frac{i}{2} \log [\hbar k]$$

$$iS_{1} = -\frac{1}{2} \log [\hbar k] = \log (\hbar k)^{-1/2},$$

$$e^{iS_{1}} = (\hbar k)^{-1/2}. \qquad ...(117)$$

and

We thus obtain to this order of approximation,

$$\psi_{WKB}(x) = A \left(\hbar k \right)^{-1/2} \exp \left(\pm i \int_{x_0}^x k \, dx \right)$$

$$= A \left[2m \left(E - V \right) \right]^{-1/4} \exp \left\{ \pm \frac{i}{\hbar} \int_{x_0}^x \left[2m \left(E - V \right) \right] \, dx \right\}.$$
...(118)

In a similar fashion, the approximate solution for the case V(x) > E is found to be

$$\psi_{WKB}(x) = A \left[2m \left(V - E \right) \right]^{-1/6} \exp \left\{ \pm \frac{1}{\hbar} \int_{x_0}^{x} \left[2m \left(V - E \right) \right] dx \right\}.$$
 (119)

The accuracy of these WKB solutions is measured by the convergence of the series for S. If the magnitude of the successive terms S_0 , $\hbar S_1$ etc. falls off rapidly the series will be convergent. Since S_0 is a monotonically increasing function of x, the ratio $\hbar S_1/S_0$ will be small if $\hbar S_1'/S_0'$ is small. We thus expect eqn. (118) to be useful in that part of the domain of x where

$$\left|\frac{\hbar S_1'}{S_0'}\right| = \left|\frac{k'}{2k^2}\right| < < 1.$$
 ...(120)

The de Broglie wavelength at the point x is given by $\lambda = 2\pi/k(x)$, so that (120) can be written as

$$\frac{\lambda}{4\pi} \left| \frac{dk}{dk} \right| < < k \qquad \dots (121)$$

Thus the change in k over the distance $\lambda/4\pi$ is much smaller than unity. Hence the WKB approximation is best when the potential function changes so slowly with position that the momentum $(\hbar k)$ of the particle is sufficiently constant over many wavelengths.

8.9. WAVEFUNCTION, FOR A PARTICLE IN A GIVEN POTENTIAL WELL AND THE QUANTIZATION RULE:

We now consider the problem of finding the wavefunction for a particle in a given potential well V(x) as shown in the fig. 2

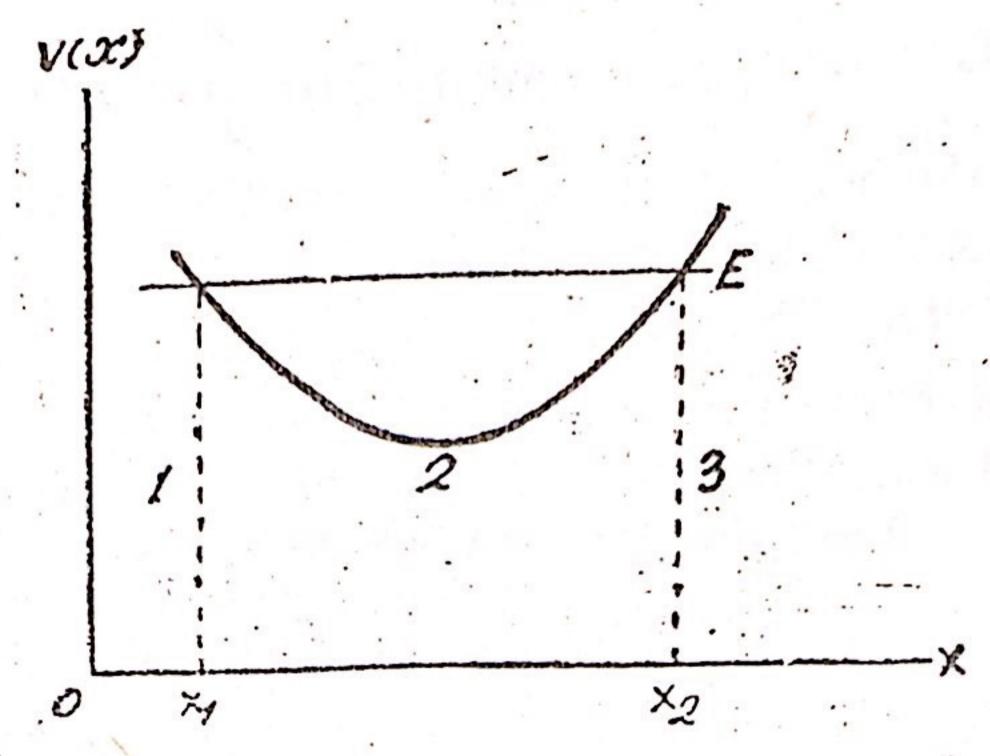


Fig. 2 Potential well.

In the first region, the wavefunction decreases exponentially as $x \to -\infty$, since V(x) > E and k(x) is imaginary, we can approximate the wavefunction ψ by

$$\psi_1 = \frac{C_1}{\sqrt{\{|k(x)|\}}} \exp\left(-\int_x^{x_1} |k(x)| dx\right), \dots (122)$$

where C₁ is an arbitrary constant.

In the region 2, ψ is oscillatory, and is given by

$$\psi_{2} = \frac{C_{2}}{\sqrt{\{k(x)\}}} \exp. \left(i \int_{-\infty}^{x} k \, dx \right) + \frac{C'_{2}}{\sqrt{\{k(x)\}}} \exp\left(-i \int_{-\infty}^{x} k \, dx \right). \tag{123}$$

In region 3, the wavefunction decreases exponentially as $x \to \infty$

$$\psi_3 = \frac{C_3}{\sqrt{\{|k(x)|\}}} \exp\left(-\int_{x_2}^x |k| dx\right). \qquad ...(124)$$

In the above C_2 , C_2 and C_3 are arbitrary constants.

Now, the above solutions fail in the immediate neighbourhood of the points x_1 and x_2 (turning points), of course, these are valid at points sufficiently remote from x_1 and x_2 . Hence we are confronted with he problem of finding ψ in the immediate neighbourhood of the points x_1 and x_2 , and matching these in the regions to the left and to the right of these points to form a continuous solution. For this we assume that the potential energy function is approximately linear in the neighbourhood of x_1 and x_2 . Thus, we write,

$$V(x) \approx E - A(x - x_1)$$
, near x_1 ; ...(125)

 $V(x) \approx E + B(x - x_2)$, near x_2(126)

and Therefore, in the neighbourhood of x_1 , the Schroedinger equation can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2mA}{\hbar^2} (x - x_1) \psi = 0 \qquad ...(127)$$

and near x_2 , it can be written as

$$\frac{d^2\psi}{dx^2} - \frac{2mB}{\hbar^2} (x - x_2) \psi = 0. \qquad ...(128)$$

Now we change the variable in equation (127) as

$$z = -\left(\frac{2mA}{\hbar^2}\right)^{1/3}(x-x_1),$$

then

$$\frac{d\psi}{dx} = \frac{d\psi}{dz} \cdot \frac{dz}{dz} = \frac{d\psi}{dz} \cdot \left\{ -\left(\frac{2mA}{\hbar^2}\right)^{1/3} \right\}$$

and

$$\frac{d^{2}\psi}{dx^{2}} = \frac{d}{dz} \left[\frac{d\psi}{dz} \left\{ -\left(\frac{2mA}{\hbar^{2}}\right)^{1/3} \right\} \right] \frac{dz}{dx} = \left(\frac{2mA}{\hbar^{2}}\right)^{2/3} \frac{d^{2}\psi}{dz^{2}}$$

Using these expressions in eqn. (127) we obtain

$$\frac{d^2\psi}{dz^2} - z\psi = 0. ...(129)$$

Similarly the substitution

$$z = \left(\frac{2mB}{\hbar^2}\right)^{1/3} (x - x_2) \qquad ...(130)$$

reduces equation (128) into equation (129).

Solutions of the differential equation (129) are the Airy functions. We require a function which vanishes asymptotically for large positive z (z > 0 corresponds to $x < x_1$ and $x > x_2$). Such a function is

$$Ai(z) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{s^3}{z} + sz\right) ds, \qquad \dots (131)$$

which has the asymptotic forms

ch has the asymptotic forms
$$Ai(z) \xrightarrow{-} \xrightarrow{+} \frac{1}{2\sqrt{(\pi)}} \frac{1}{z^{1/4}} \exp\left(-\frac{2}{3}z^{3/2}\right); (z > 0),...(132)$$

$$Ai(z) \xrightarrow{z \to -\infty} \frac{1}{\sqrt{(\pi)(-z)^{1/4}}} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right]; (z < 0).$$
 ...(133)

In the neighbourhood of x_1 , we have

$$[k(x)]^{2} \approx \frac{2mA(x-x_{1})}{\hbar^{2}} = -\left(\frac{2mA}{\hbar^{2}}\right)^{2/3} z.$$

$$\int_{x_1}^{x} |k(x)| dx = \left(\frac{2mA}{\hbar^2}\right)^{1/3} \int_{x_1}^{x} \sqrt{(z)} dx = -\int_{0}^{x} \sqrt{(z)} dz = -\frac{2}{3}z^{3/2} \dots (134)$$

and $\int_{x_1}^{x} k(x) dx = \left(\frac{2mA}{\hbar^2}\right)^{1/3} \int_{x_1}^{x} \sqrt{(-z)} dx = -\int_{0}^{z} \sqrt{(-z)} dz = \frac{2}{8} (-z)^{3/2}.$...(135)

Comparison of these equations with equation 132 and (133) shows that the function approximated on the left of x_1 by

$$\psi_1 \approx \frac{1}{\sqrt{\{k(x)\}}} \exp\left(\int_{x_1}^{x} |k(x)| dx\right); x < x_1 \dots (136)$$

can be approximated on the right of x_1 by

$$\psi \approx \frac{2}{\sqrt{\{k(x)\}}} \sin \left[\int_{x_1}^{x} k(x) \, dx + \frac{\pi}{4} \right]; x > x_1 \quad ...(137)$$

A similar analysis in the neighbourhood of point x_2 shows that the function approximated on the right of x_2 by

$$\psi_3 \approx \frac{1}{\sqrt{\{k(x)\}}} \exp \left\{-\int_{x_3}^x |k(x)| dx\right\}, x > x_2 \dots (138)$$

can be approximated on the left of x_2 by

$$\psi \approx \frac{2}{\sqrt{\{k(x)\}}} \sin \left[\int_{x}^{x_2} k(x) dx + \frac{\pi}{4} \right], x < x_2 ... (139)$$

Functions (137) and (139) are the continuations of ψ_1 and ψ_3 ; respectively, in the region 2. Therefore, the functions given by eqns. (137) and (139), both of which define the wavefunction for the same region 2, may differ from each other, at most, by a constant multiplier; because they represent the same quantum mechanical state. Thus we have

$$\sin \left[\int_{x_1}^{x} k(x) \, dx + \frac{\pi}{4} \right] = C \sin \left[\int_{x}^{x_2} k(x) \, dx + \frac{\pi}{4} \right]$$
or
$$\sin \left[\int_{x_1}^{x_2} k(x) \, dx - \int_{x}^{x_2} k(x) \, dx + \frac{\pi}{4} \right] = C \sin \left[\int_{x_1}^{x_2} k(x) \, dx + \frac{\pi}{4} \right]$$

This condition can be satisfied only if

$$\int_{x_1}^{x_2} k(x) dx = \left(n + \frac{1}{2} \right) \pi \quad (n \text{ an integer}); \quad ...(140)$$

Constant C is then equal to $(-1)^n$ and the unnormalized WKB approximation to the bound state wavefunction is given by

$$\psi_{WKB} = \begin{cases}
\frac{(-1)^n}{\sqrt{\{ \mid k(x) \mid \}}} \exp \left\{ -\int_x^{x_1} \mid k(x) \mid dx \right\} (x < x_1) \\
\frac{2 (-1)^n}{\sqrt{\{ k(x) \}}} \sin \left[\int_{x_1}^x k(x) dx + \frac{\pi}{4} \right] (x_1 < x < x_2) \dots (141) \\
\frac{1}{\sqrt{\{ \mid k(x) \mid \}}} \exp \left\{ -\int_{x_1}^x \mid k(x) \mid dx \right\} (x > x_2)
\end{cases}$$

Substituting the expression (109) for k into (140), we obtain

$$2\int_{x_1}^{x_2} \{2m \left[E-V(x)\right]\}^{1/2} dx = (n+\frac{1}{2}) h, n=0, 1, 2, \dots (142)$$

The left hand side is just $\oint pdx$, i.e. the integral of the momentum of a classical particle over one complete cycle of its motion from x_1 to x_2 and back to x_1 . Thus eqn. (142) is the **Bohr-Sommerfeld** quantum rule, with the difference that instead of an integer quantum number, the half integer $(n+\frac{1}{2})$ appears here.

8.10. APPLICATION OF W.K.B.—TRANSMISSION THROUGH A POTENTIAL BARRIER:

We have solved the Schroedinger equation for the simple case of penetration through a square potential barrier. For a barrier of more complicated shape, in general, the Schroedinger equation can not be solved exactly. However, we can find an approximate solution of the equation for any form of the potential barrier by using the WKB-method.

Let us consider the case of the barrier of arbitrary shape as shown in Fig. 3. In region 2, energy of the particle is less

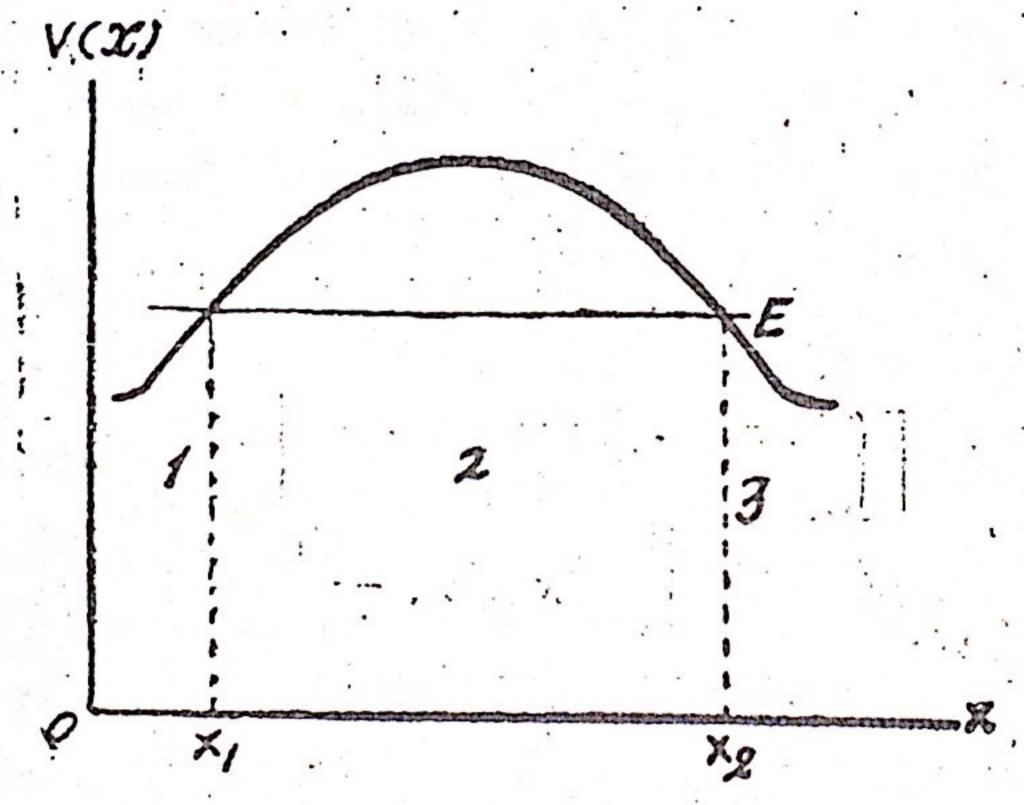


Fig. 3. Potential Barrier

than the potential barrier and hence the particle cannot exist in this region according to the classical mechanics. However, we know that the particle can penetrate the barrier and there is a finite probability of finding the particle into region 3; according to quantum mechanics. From WKB approximation we know that the wave-function is oscillatory outside the barrier and has exponential character in the non-classical region. In the

wavefunction (141), the exponentially increasing solution in the regions 1 and 3 was discarded because it violates the boundary conditions for ψ at $x \to \pm \infty$. In the present case, however, the exponential character of the solution in region 2 will include both exponential solutions, as the region 2 is of finite width. Hence we can write for the regions 1 and 3,

$$\psi_{1} = \frac{C_{1}}{\sqrt{\{k(x)\}}} \exp \left\{ i \int_{x}^{x_{1}} k(x) dx \right\} ...(143)$$

$$\psi_{3} = \frac{C_{3}}{\sqrt{\{k(x)\}}} \exp \left\{ i \int_{x_{2}}^{x} k(x) dx \right\} \dots (144)$$

and for region 2, we write

$$\psi_{2} = \frac{C_{2}}{\sqrt{\{|k(x)|\}}} \exp \left\{ \int_{-\infty}^{x} |k(x)| dx \right\} + \frac{C'_{2}}{\sqrt{\{k(x)\}}} \exp \left\{ -\int_{-\infty}^{x} |k(x)| dx \right\} ...(145)$$

As in the last section, here also, these solutions fail near the turning points x_1 and x_2 . We require therefore a second connection formula. We use the second solution of the differential equation (129), which is the Airy function

$$Bi(z) = \frac{1}{\pi} \int_0^\infty \left[\exp\left(-sz - \frac{1}{2}s^3\right) + \sin\left(\frac{s^3}{3} + sz\right) \right] ds. \qquad \dots (146)$$
with the asymptotic forms

$$Bi(z) \sim \frac{1}{\sqrt{(\pi)z^{1/4}}} \exp \left[\frac{2}{3} z^{3/2}\right] (z > 0)$$
 ...(147)

$$Bi(z) \sim \frac{1}{\sqrt{(\pi)(-z)^{1/4}}} \cos \left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right], (z < 0) \dots (148)$$

Like preceding section approximating the potential function by a linear function near the turning points (see fig. 4), the con-

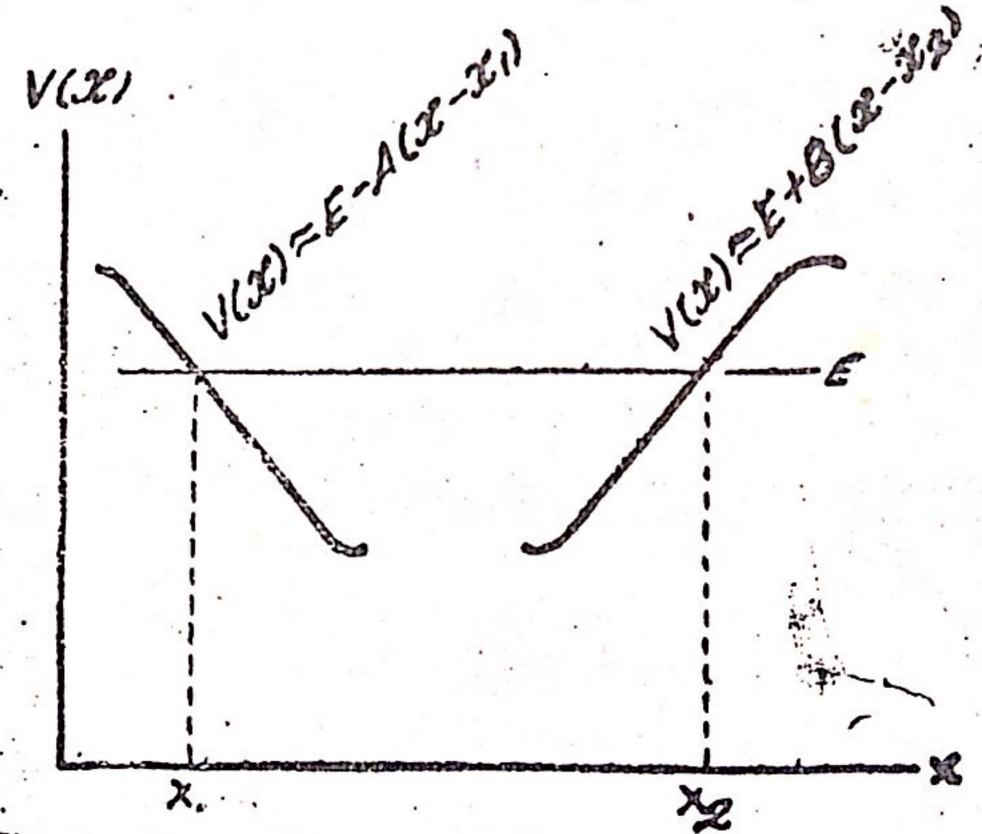


Fig. 4. Potentials near the turning points x_1 and x_2

nection formula linking an increasing exponential solution in region 1 to an oscillatory solution in region 2 is given as:

$$\psi_{WKB} = \begin{cases} \frac{1}{\sqrt{\{k(x)|\}}} & \exp\left\{\int_{x}^{x_{1}} |k(x)| dx\right\} (x < x_{1}), \\ \frac{1}{\sqrt{\{|k(x)|\}}} & \cos\left[\int_{x_{1}}^{x} k(x) dx + \frac{\pi}{4}\right] (x > x_{1}). \\ \dots (149) \end{cases}$$

In order to facilitate the application of (149), we write the wavefunction for the transmitted particle [(eqn. (144)] in the form:

$$\psi_3 = \frac{A}{\sqrt{\{k(x)\}}} \exp. i \left[\int_{x_2}^x k(x) \, dx \frac{\pi}{4} \right] (x > x_2) \qquad \dots (150)$$

In terms of trigonometric functions we can write it as

$$\psi_{3} = \frac{A}{\sqrt{\{k(x)\}}} \left\{ \cos \left[\int_{x_{2}}^{x} k(x) dx + \frac{\pi}{4} \right] + i \sin \left[\int_{x_{2}}^{x} k(x) dx + \frac{\pi}{4} \right] \right\}. \dots (151)$$

Comparing eqn. (151) with eqs. (141) and (149), we get the connecting wavefunction of exponential type for region 2 as

$$\psi_{2} = \frac{A}{\sqrt{\{|k(x)|\}}} \left[\exp \left(\int_{x}^{x_{2}} |k(x)| dx \right) + \frac{i}{2} \exp \left(-\int_{x}^{x_{2}} |k(x)| dx \right) \right] \dots (152)$$

Now splitting the integral as:

$$\int_{x}^{x_{2}} = \int_{x_{1}}^{x_{2}} - \int_{x_{1}}^{x}$$

and introducing the notation

$$J = \exp\left(-\int_{x_1}^{x_2} |k(x)| dx\right),$$
 ...(153)

we can write eqn. (152) as:

$$\psi_{2} = \frac{A}{\sqrt{\{|k(x)|\}}} \left[\frac{1}{J} \exp \left(-\int_{x_{1}}^{x} |k(x)| dx \right) + \frac{iJ}{2} \exp \left(\int_{x_{1}}^{x} |k(x)| dx \right) \right] \qquad \dots (154)$$

Comparing eqn. (154) with eqns. (149) and (141), the connecting oscillatory wavefunction in region 1 is now found to be

$$\psi_{1} = \frac{A}{\sqrt{\{k(x)\}}} \left[\frac{2}{J} \sin \left(\int_{x}^{x_{1}} k(x) dx + \frac{\pi}{4} \right) + \frac{iJ}{2} \cos \left(\int_{x}^{x_{1}} k(x) dx + \frac{\pi}{4} \right) \right] \dots (155)$$

Writing it in terms of exponentials

$$\psi_{1} = \frac{A}{i\sqrt{\{k(x)\}}} \left\{ \left(\frac{1}{J} - \frac{1}{4} J \right) \exp \left[i \left(\int_{x}^{x_{1}} k(x) dx + \frac{\pi}{4} \right) \right] - \left(\frac{1}{J} + \frac{1}{4} J \right) \exp \left[-i \left(\int_{x}^{x_{1}} k(x) dx + \frac{\pi}{4} \right) \right] \right\} \dots (156)$$

The first term in the braces is a wave moving to the left, and hence represents the reflected wave, while the second term represents the incoming wave, which moves to the right.

The transmission coefficient is the ratio of transmitted to incident wave amplitudes.

Transmission coefficient,

$$T = \frac{\left| \frac{A}{i\sqrt{\{k(x)\}}} \left(\frac{1}{J} + \frac{1}{4}J \right) \exp\left[-i\left(\int_{x}^{x_{1}} k(x) dx + \frac{\pi}{4} \right) \right] \right|^{2}}{\left| \frac{A}{\sqrt{\{k(x)\}}} \exp\left[i\left[\int_{x_{2}}^{x} k(x) dx + \frac{\pi}{4} \right] \right]^{2}} = \frac{J}{1 + \frac{J^{2}}{4}} \qquad \dots (157)$$

In the WKB approximation, we can neglect the powers of J higher than the first, because these terms involve square and higher powers of \hbar . Therefore,

$$T \approx J = \exp\left\{-\int_{x_1}^{x_2} |k(x)| dx\right\}$$

$$= \exp\left\{-\frac{1}{\hbar} \int_{x_1}^{x_2} \sqrt{2m \left[V_{\ell}(x) - E\right]} dx\right\} \dots (158)$$

8.11. RADIATION THEORY—AN APPLICATION OF HARMONIC PERTURBATION

In this part we shall discuss the effect of electromagnetic radiations on the atomic electrons by treating the interaction between the radiation and the electron in an atom as a small perturbation. We begin with a discussion of the terms like induced and spontaneous emissions.

Let us consider an atomic system having two energy levels E_1 and E_2 ($E_2 > E_1$). The system emits a photon of frequency ν given by $E_2 - E_1 = h\nu$ when it falls from state 2 to state 1, and it will absorb a photon of the same frequency when it is excited from the state 1 to 2. The transitions from state 1 to 2 and from state 2 to 1 are caused by the interaction with the external radiation.

If N_1 atoms are in the ground state and N_2 atoms are in the higher state, then the total number of atoms

$$N = N_1 + N_2 = Constant$$
 ...(159)

Now suppose that $\rho(v)$ is the energy density of the radiation interacting with the atomic system, then the energy per unit volume in the frequency range v to v+dv is defined by $\rho(v) dv$. In terms of this definition of energy density, Einstein assumed that the probability of transition for the atoms in state E_2 to a lower energy state E_1 , by emitting a photon of frequency v, is given by $B \rho(v)$. Here B is known as Einstein's coefficient for the emission of photons. Similarly, the probability of absorption is given by $B \rho(v)$. Hence, $N_1 B \rho(v)$ atoms will rise per second from state 1 to state 2, and $N_2 B P(v)$ atoms will fall per second from state 2 to 1. Therefore, the net rate of decrease of atoms from state 1 is given by

$$\frac{dN_1}{dt} = -N_1 B \rho(v) + N_2 B \rho(v). \qquad ...(160)$$

The negative sign signifies that the atoms in the state 1 are decreasing.

Using eqn. (159) into eqn. (160), we can eliminate N₂ from eqn. (160). We get

$$\frac{dN_1}{dt} = -N_1 B \rho(v) + (N - N_1) B \rho(v) - \frac{dN_1}{dt} = (2N_1 - N) B \rho(v).$$

of

Integrating this equation, we get

$$\frac{1}{2}\log_{0}(2N_{1}-N)=-B\rho(v)t+C.$$

To find the constant of integration C, we use the initial condition that at time t=0, all the atoms are in the ground state, i.e. $N_1 = N$ at t = 0. Therefore

 $\frac{1}{2}\log_{\theta}(2N-N)=C \Rightarrow C=\frac{1}{2}\log_{\theta}N$

and hence, we have

or
$$\frac{1}{2} \log_{\theta} (2N_1 - N) = -B \rho(v) t + \frac{1}{2} \log_{\theta} N$$

or $\frac{1}{2} \log_{\theta} \left(\frac{2N_1 - N}{N}\right) = -B \rho(v) t$
or $\frac{2N_1 - N}{N} = e^{-2B \rho(v) t}$

or

 $N_1 = \frac{1}{2}N \{1 + e^{-2B} \rho(v) t\}$

This gives the number of atoms in the ground state at any

time t. It is clear that as the time increases, the exponential factor in (161) decreases and hence the number of atoms in the ground state will decrease. After very long time $(t=\infty)$, we have $N_1 = \frac{1}{2}N$(162)

Thus half of the total number of atoms are in the ground state and half of them are in the upper state. But the number of atoms in the upper state should be lesser because the atoms prefer to be in their more stable ground state. In order to explain this, Einstein introduced the concept of Spontaneous emission. He gave the idea that the emission of photons may take place even in the absence of all external radiations. This type of emission is known as the spontaneous emission. The absorption and the emission of radiation in the presence of an external field is known as the Induced absorption and the Induced emission: respectively.

Probability of spontaneous emission is denoted by A, called the *Einstein's coefficient* of spontaneous emission. Hence the rate of decrease of atoms from the ground state is given by

$$\frac{dN_1}{dt} = -N_1 B \rho(v) + N_2 \{A + B \rho(v)\}. \qquad ...(163)$$

For the steady state case, N_1 and N_2 are fixed. Therefore we have $\frac{dN_1}{dt} = 0$, and hence

$$-N_1 B \rho(\nu) + N_2 \{A + B \rho(\nu)\} = 0$$

$$\frac{N_2}{N_1} = \frac{B \rho(\nu)}{A + B \rho(\nu)} = \frac{1}{\frac{A}{B} \cdot \frac{1}{\rho(\nu)} + 1} \cdot \dots (164)$$

or

From Planck's law of radiation, energy per unit volume in the frequency range v to v+dv is given by

$$\rho(v) \ dv = \frac{8\pi v^3 h}{c^3} \cdot \frac{dv}{e^{kv/kT} - 1}.$$
 ...(165)

Also, from thermodynamics, for the steady state case we have

$$\frac{N_2}{N_1} = \frac{e^{-E_2/kT}}{e^{-E_1/kT}} = e^{-(E_2 - E_1)/kT} = e^{-h\nu/kT}. \qquad ...(166)$$

From eqns. (164) and (166), we can write

$$\frac{e^{-h\nu/kT}}{B} = \frac{1}{\frac{A}{B} \cdot \frac{1}{\rho(\nu)} + 1}$$

or.
$$\frac{A}{B} = \rho(v) [e^{hv/kT} - 1].$$
 ...(167)

Using the value of p(v) from eqn. (165) into it we get

$$\frac{A}{B} = \frac{8\pi v^3 h}{c^3} \cdot \frac{1}{e^{hv/kT} - 1} \cdot (e^{hv/kT} - 1) = \frac{8\pi v^3 h}{c^3}. \qquad ...(168)$$

INTERACTION OF RADIATION WITH ATOM:

The Hamiltonian for an atom in the absence of radiation field can be written as

$$H_0 = \frac{p^2}{2m} + V(r).$$
 ...(169)

If the atom is placed in an electromagnetic field characterized by the vector potential A and scalar potential ϕ , the interaction can be introduced by the standard prescription $p \rightarrow p - \frac{e}{c} A$; $V(r) \rightarrow V(r) + e\phi$. Hence the Hamiltonian for the atom in the presense of the radiation field can be written as.

Sense of the rank

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^{2} + V(r) + e\phi$$

$$= \frac{1}{2m} \left(\mathbf{p}^{2} + \frac{e^{2}}{c^{2}} \mathbf{A}^{2} - \frac{e}{c} \mathbf{p} \cdot \mathbf{A} - \frac{e}{c} \mathbf{A} \cdot \mathbf{p} \right) + V(r) + e\phi$$

$$= \frac{\mathbf{p}^{2}}{2m} + V(r) - \frac{e}{2mc} \left(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p} \right) + \frac{e^{2}}{2mc^{2}} \mathbf{A}^{2} + e\phi. \quad ...(170)$$

Now $(\mathbf{p} \cdot \mathbf{A})_x \psi = p_x A_x \psi = -i\hbar \frac{\partial}{\partial x} (A_x \psi)$ $=-i\hbar\,\frac{\partial A_x}{\partial x}\,\psi-i\hbar\,A_x\,\frac{\partial\psi}{\partial x}$ $= (p_x A_x) \psi + A_x (p_x \psi).$

$$p \cdot A = -i\hbar \nabla \cdot A + A \cdot p.$$

Using it into eqn. (170), we get.

Using it into eqn. (170), we get
$$H = \frac{\mathbf{p}^2}{2m} + V(r) + \frac{i\hbar e}{mc} \mathbf{A} \cdot \nabla + \frac{e^2}{2mc^2} \mathbf{A}^2 + \frac{i\hbar e}{2mc} (\nabla \cdot \mathbf{A}) + e\phi.$$

We can use the Gauge transformation of first kind to make $\nabla \cdot A = 0$ and $\phi = 0$. Then we have

nd
$$\phi = 0$$
. Then we have $H = \frac{\mathbf{p}^2}{2m} + V(r) + \frac{i\hbar e}{mc} \mathbf{A} \cdot \nabla + \frac{e^2}{2mc^2} \mathbf{A}^2$.

For the first order theory, second order term, $e^2A^2/2mc^2$, in H can be neglected and hence we have

ed and hence we have
$$i\hbar e$$
 and $H = H_0 + H'$; $H' = \frac{i\hbar e}{mc} \mathbf{A} \cdot \nabla$(171)

For a weak field, H' can be regarded as a small perturbation to the Hamiltonian H_0 .

Now the plane wave expression for A with propagation vector k and angular frequency $\omega = |\mathbf{k}| c$ is given by

$$A = 2A_0 \cos(k \cdot r - \omega t + \alpha)$$

 $=A_0' \exp [i (k \cdot r - \omega t)] + A_0'^* \exp [-i (k \cdot r - \omega t)], ...(172)$ where $A_0' = A_0 e^{i\alpha}$ is a constant real vector and α is an arbitrary (real) phase constant.

In order to satisfy the condition $\nabla \cdot A = 0$ for A given by eqn. (172), we should have $A_0 \cdot k = 0$.

Using eqn. (172) in H', we can express the perturbation part as

$$H' = H_0' e^{-i\omega t} + H_0'' e^{i\omega t}, \text{ where}$$

$$H_0' = \frac{i\hbar e}{mc} e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{A}_0' \cdot \nabla, \text{ and } H_0'' = \frac{-i\hbar e}{mc} e^{-\mathbf{k} \cdot \mathbf{r}} \mathbf{A}_0' \cdot \nabla.$$
...(173)

Using this value of H' into equation (56), the first order amplitude for a transition from the initial state n to final state k is given by

$$a_{k}(t) = -\frac{\langle k \mid H_{0} \mid n \rangle}{\hbar} \cdot \frac{e^{i (\omega_{kn} - \omega)} t}{(\omega_{kn} - \omega)}$$

$$-\frac{\langle k \mid H_{0}'' \mid n \rangle}{\hbar} \cdot \frac{e^{i (\omega_{kn} + \omega)} t}{(\omega_{kn} + \omega)}, \dots (174)$$

where

$$\langle k \mid H_0' \mid n \rangle = \frac{i\hbar e}{mc} \int \psi_k^{(0)*} e^{i\mathbf{k} \cdot \mathbf{r}} A_0' \cdot \nabla \psi_n^{(0)} d^3r$$
and $\langle k \mid H_0'' \mid n \rangle = \frac{i\hbar e}{mc} \int \psi_k^{(0)*} e^{-i\mathbf{k} \cdot \mathbf{r}} A_0^* \cdot \nabla \psi_n^{(0)} d^3r$

$$\dots(175)$$

Functions $\psi_n^{(0)}$ are the eigenfunctions of the unperturbed Hamiltonian H_0 , and ∇_{A_0} is the component of ∇ along A_0

The first term on the right hand side of eqn. (174) gives rise to upward transitions $(E_k^{(0)} > E_n^{(0)})$ with a probability proportional to $|\langle k | H_0' | n \rangle|^2$, provided $\hbar \omega = E_k^{(0)} - E_n^{(0)})$. The second term probability generates downward transitions $(E_k^{(0)} < E_n^{(0)})$ with proportional to $|\langle k | H_0'' | n \rangle|^2$ if $\hbar \omega = E_n^{(0)} - E_k^{(0)}$. In making an upward transition, the system absorbs a quantum $\hbar \omega$ of radiation energy from the electromagnetic field, and that in a downward transition it emits a quantum of energy $\hbar \omega$.

A constant transition probability per unit time is obtained if the incident radiation is monochromatic and transition can occur to any of a group of closely spaced states. However, the computation of a transition probability between two discrete states is often of interest. For it we assume that the radiation covers a spread of frequency $\Delta \omega$ with no relation between the different frequency components, so that the radiations can be characterized by a density of waves per unit frequency range.

Hence the probability of absorption of a photon of energy $\hbar \omega$ at time t is given by

$$a_{k}(t) \mid^{2} = \sum_{\omega} \frac{4 \mid \langle k \mid H_{0}' \mid n \rangle \mid^{2} \sin^{2} \frac{1}{2} (\omega_{kn} - \omega) t}{\hbar^{2} (\omega_{kn} - \omega)^{2}}$$

$$= \sum_{\omega} \frac{4e^{2}\hbar^{2}}{m^{2}c^{2}} \mid A_{0}' \mid^{2} \mid \int \psi_{k}^{(0)*} e^{i\mathbf{k} \cdot \mathbf{r}} \nabla_{A_{0}'} \psi_{n}^{(0)} d^{3}r \mid^{2}$$

$$\times \frac{\sin \frac{1}{2} (\omega_{kn} - \omega) t}{\hbar^{2} (\omega_{kn} - \omega)^{2}} \dots (176)$$

Now the electric and the magnetic fields associated with the vector potential (172) is given by

$$\mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} = -2k \mathbf{A}_0 \sin (\mathbf{k} \cdot \mathbf{r} - \omega t + \alpha) \quad [:: \phi = 0 \text{ and } \omega = kc]$$
and $\mathbf{B} = \mathbf{V} \times \mathbf{A} = -2k \times \mathbf{A}_0 \sin (\mathbf{k} \cdot \mathbf{r} - \omega t + \alpha)$(177)

Therefore, the contribution of the wave (172) to the instantaneous energy density is given by the Poynting vector

$$P = \frac{c}{4\pi} E \times B = \frac{c}{4\pi} \cdot 4k^2 A_0^2 \sin^2(k \cdot r - \omega t + \alpha),$$

where we have used the fact that A_0 is perpendicular to k. Its value averaged over one period $2\pi/\omega$ is $\omega^2 A_0^2/2\pi c$. Hence the intensity in Bohr frequency range $\Delta \omega$ is given by

$$I(\omega) \triangle \omega = \frac{\omega^2}{2\pi c} A_0^2 = \frac{\omega t}{2\pi c} A_0'^2 \quad \{ :: \quad A' \mid = \mid A_0 \mid \}.$$

$$\therefore \quad A_0'^2 = \frac{2\pi c}{\omega^2} I(\omega) \triangle \omega. \qquad \dots (178)$$

Using this into eqn. (176), we have

$$|a_k(t)|^2 = \sum_{m^2 c \omega^2} \frac{8\pi e^2}{m^2 c \omega^2} I(\omega) \triangle \omega \left| \int \psi_k^{(0)} e^{i\mathbf{k} \cdot \mathbf{r}} \nabla_{A_0} \psi_n^{(0)} d^{3r} \right|^2$$

$$\times \frac{\sin \frac{1}{2} (\omega_{kn} - \omega) t}{\hbar^2 (\omega_{kn} - \omega)^2}.$$

If the frequency range $\Delta \omega$ is made infinitesimally small, then summation may be replaced by integration, because the contribution

due to different frequency components is additive one. Thus the transition probability per unit time for an upward transition is

Isition probability por any
$$\frac{|a_k(t)|^2}{t} = \frac{8\pi e^2}{m^2 c \omega^2_{kn}} I(\omega_{kn}) \left| \int \psi_k^{(0)*} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_0} \psi_n^{(0)} d^{8r} \right|^2 \times \int_{-\infty}^{+\infty} \frac{\sin \frac{1}{2} (\omega_{kn} - \omega)t}{(\omega_{kn} - \omega)^2 t} d\omega$$

Since the time factor has a sharp maximum at $\omega = \omega_{kn}$, the other factors having ω are taken outside.

Evaluating the integral in the above, we get

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$$\frac{|(a_k(t))|^2}{t} = \frac{4\pi^2 e^2}{m^2 c \omega^2_{kn}} I(\omega_{kn}) \left| \int \psi_k^{(0)*} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_0} \psi_n^{(0)} d^3r \right|^2 \dots (179)$$

Similarly, the transition probability for the emission of a photon of energy $\hbar \omega$ is given by

$$\frac{|a_{k'}(t)|^{2}}{t} = \frac{4\pi^{2}e^{2}}{m^{2}c\omega^{2}nk'}, I(\omega_{nk'}) \left| \int \psi_{k'}^{(0)*} e^{-i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_{0'}} \psi_{n}^{(0)} d^{3}r \right|^{2} \dots (180)$$

This can be made to describe the transition from an initial upper state k to a final lower state n, if n is replaced by k and k' by n. Therefore,

$$\frac{|a_n(t)|^2}{t} = \frac{4\pi^2 e^2}{m^2 c \omega_{kn}^2} I(\omega_{kn}) \int \psi_n^{(0)} e^{-i\mathbf{k} \cdot \mathbf{r}} \nabla_{A_0} \psi_k^{(0)} d^3 r \Big|^2 ...(181)$$

Because ∇_{A_0} , is along the vector A_0 which is perpendicular to k, we have

$$\int \psi_{n}^{(0)*} e^{-i\mathbf{k} \cdot \mathbf{r}} \nabla_{A_{0}} \psi_{k}^{(0)} d^{3}r = \left(\int \psi_{k}^{(0)} e^{i\mathbf{k} \cdot \mathbf{r}} \nabla \dagger_{A_{0}} \psi_{n}^{(0)} d^{3}r \right)^{*}$$

$$= -\int \psi_{k}^{(0)*} e^{i\mathbf{k} \cdot \mathbf{r}} \nabla_{A_{0}} \psi_{n}^{(0)} d^{3}r \qquad \dots (182)$$

From this we see that the square of the magnitude of the integral in eqn. (181) is the same as of the integral appearing in eqn. (179). Thus we conclude that the upward transition probability per unit time is the same as the downward transition probability per unit time and it is given by

$$\frac{4\pi^{2}e^{2}}{m^{2}c\omega^{2}_{kn}}I(\omega_{kn})\left|\int \psi_{k}^{(0)} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_{0}} \psi_{n}^{(0)} d^{3}r\right|^{2} \dots (183)$$

8.13. ELECTRIC DIPOLE TRANSITIONS:

We have seen that the transition probability per unit time for a transition between the two states n (lower) and k (upper) is

or

given by equation (183). In most of the cases of practical interest, the wavelength of the radiation is many times greater than the linear dimension of the atom. For example, for visible light, $\lambda \approx 10^{-5}$ cms and r = size of the atom $\approx 10^{-8}$ cms. Thus

$$\lambda \propto \frac{1}{k} > r \Rightarrow kr < < 1.$$
 ...(184)

Hence a good appoximation is obtained by replacing,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 1 + i\mathbf{k}\cdot\mathbf{r} + \frac{1}{2}(i\mathbf{k}\cdot\mathbf{r})^2 + \dots$$

in the integral of eqn. (183) by the leading term, i.e., unity. This is known as the Long-wavelength or Dipole approximation. Under this approximation, we can write the transition probability as

$$\frac{4\pi^{2}e^{2}}{m^{2}c\omega_{kn}^{2}}I(\omega_{kn})\left|\int_{k}^{(0)} \psi_{k}^{(0)} \nabla_{A_{0}} \psi_{n}^{(0)} d^{3}r\right|^{2} ...(185)$$

Now
$$H_0 \mathbf{r} - \mathbf{r} H_0 = -\frac{i\hbar}{m} \mathbf{p} = -\frac{\hbar^2}{m} \nabla$$

$$: \langle k | (H_0 \mathbf{r} - \mathbf{r} H_0) | n \rangle = -\frac{\hbar^2}{m} \langle k | \nabla | n \rangle$$

or
$$\left(E_k^{(0)} - E_n^{(0)}\right) \langle k \mid r \mid n \rangle = -\frac{\hbar^2}{m} \langle k \mid \nabla \mid n \rangle$$

$$\hbar \omega_{kn} \langle k \mid r \mid n \rangle = -\frac{\hbar^2}{m} \langle k \mid \nabla \mid n \rangle$$

$$\Rightarrow \langle k \mid \nabla \mid n \rangle = -\frac{m}{\hbar^2} \hbar \omega_{kn} \langle k \mid r \mid n \rangle \qquad ...(186)$$

Using it into eqn. (185) we get the transition probability as

$$\frac{4\pi^2 e^2}{\hbar^2 c} I(\omega_{kn}) | < k | \mathbf{r}_{A_0} | n > |^2, \qquad ...(187)$$

where \mathbf{r}_{A_0} is the component of \mathbf{r} in the direction of \mathbf{A}_0 . If θ is the angle between \mathbf{r} and the direction of polarization of the incident radiation, then $\mathbf{r}_{A_0} = \mathbf{r} \cos \theta$, and we can write (187) as

$$\frac{4\pi^2 e^2}{\hbar^2 c} I(\omega_{kn}) |\langle k | r | n \rangle|^2 \cos^2 \theta \qquad \dots (188)$$

It is observed that this quantity does not involve the direction of polarization. Therefore it is easy to calculate the transition rate due to unpolarized radiation with all directions of proparate on. We merely have to average (188) over θ . Then we get the transition probability for the electric dipole transitions as

$$\frac{4\pi^2c^2}{3\hbar^2c}I(\omega_{kn})|\langle k|\mathbf{r}|n\rangle|^2 \qquad ...(189)$$

We call it as the dipole transition, because the matrix element of the electric dipole moment er of the particle involved in it.

8.14. SELECTION RULES AND FORBIDDEN TRANSITION:

It has been shown that the probability that a transition will occur as a sesult of electromagnetic radiation incident on an atom is proportional to the square of the matrix element of the interaction term in Hamiltonian which couples the two energy states in question. The conditions under which the matrix element is nonzero constitute the selection rules. If the potential which constitutes the unperturbed Hamiltonian is spherically symmetric, the energy eigenfunction are written as the product of radial and spherical harmonic functions, *i.e.*,

$$\psi_{nlm}^{(0)} = R_{nl}(r) P_l^m(\cos \theta) e^{im\phi}$$
 ...(190)

The three components of the dlpoie matrix element $\langle k | r | n \rangle$ can thus be written as

$$X = \int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} \psi_{n'l'm'}^{(0)*} r \sin\theta \cos\phi \psi_{nlm}^{(0)} d^{3}r \qquad ...(191a)$$

$$Y = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_{n'l'm'}^{(0)*} r \sin\theta \sin\phi \psi_{nlm}^{(0)} d^3r \qquad \dots (191b)$$

$$Z = \int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} \psi_{n'l'm'}^{(0)*} r \cos \theta \psi_{nlm}^{(0)} d^{3}r \qquad ...(191c)$$

The X-component can be written as

$$X = \int_0^\infty R_{n'l'}(r) R_{nl}(r) r^2 dr \int_0^\pi P_{l'}^{m'}(\cos \theta) \sin \theta P_{l}^{m}(\cos \theta) \sin \theta d\theta$$

$$\times \int_0^{2\pi} e^{-im'\phi} \cos \phi e^{im\phi} d\phi \qquad ...(192)$$

with cos $\phi = (e^{i\phi} + e^{-i\phi})/2$, the ϕ integral is found to be

$$\frac{1}{2} \int_{0}^{2\pi} \left[e^{i(m-m'+1)\phi} + e^{i(m-m'-1)\phi} \right] d\phi$$

$$= \begin{cases} \pi & \text{if } m'=m+1 \\ 0 & \text{otherwise} \end{cases} \dots (193)$$

Making use of the relation

$$\sin\theta P_{l'}^{m-1} = \frac{P_{l'+1}^m - P_{l'-1}^m}{2l+1} \qquad \dots (194)$$

and the result of equation (193), the orthogonality P_i^m with respect to l for equal m then leads to the result

$$\int_{0}^{\pi} P_{l'}^{m+1} \sin \theta \, P_{l}^{m} \sin \theta \, dt = 0 \text{ unless } l' = l \pm 1 \qquad \dots (195)$$

The solution of r-integral puts no restriction upon n. Similarly, the condition on Y and Z components of matrix element to zero, further leads to the following results

$$Y=0$$
 except with $m'=m\pm 1$ and $i'=l\pm 1$. $Z=0$ except when $m'=m$ and $l'=l\pm 1$. $\{196\}$

The above results constitute the ejectric dipole selction rules for atomic transitions. The selction rules allow only those transitions for which

 $\triangle l = \pm 1$ and $\triangle m = 0, \pm 1$(197) If these rules are not satisfied, then it does not mean that the transition is not occurring at all, because they may be occurring in higher dipole approximations.

If both the state $|k\rangle$ and $|n\rangle$ are spherically symmetric (e.g. $1S\rightarrow 2S$), the integral $\int_{k}^{\psi_{n}^{(0)}} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_{0}^{\prime}} \psi_{n}^{(0)} d^{3}r$ is identically zero. To see it, let us choose the coordinates in such a way the x-axis is along the direction, of polariation. Then $\Delta_{A_{0}^{\prime}} \psi_{n}^{(0)}$ is an odd function of x, whereas ψ_{k} is an even function of x. Exponential ex. $(i\mathbf{k}\cdot\mathbf{r}) = \exp[i(k_{y}y + k_{z}z)]$ is also even in x, since k perpendicular to A_{0}^{\prime} lies in the (y, z)-plane. The transition between these states is said to be strictly forbidden, because the first order probability for these transitions is [zero. However, higher order of perturbations may produce these transitions.

8 15. EINSTEIN'S A $\nabla_{A_0}, \psi_n^{(0)}$ AND B CO-EFFICIENTS:

We have seen that the transition probability per unit time for the absorption and emission of radiations is given by

$$\frac{|a_k(t)|^2}{t} = \frac{4\pi^2 e^2}{m^2 c\omega^2} I(\omega) |\langle k|e^{i\mathbf{k}\cdot\mathbf{r}} \Delta_{A_0}, |n\rangle^2 \qquad \dots (198)$$

The Einstein's B coefficient is also related with the probability of induced emission and absorption. Therefore, we can relate (198) with the B coefficient. If $\rho(\omega)$ is the identity of the radiation per unit angular frequency range, then

$$\rho(\omega) d\omega = \frac{I(\omega) d\omega}{c}$$

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$$\therefore \quad \rho(\omega) = \frac{I(\omega)}{c}$$

Hence we have

Hence we have
$$\frac{|a_k(t)|^2}{t} = \frac{4\pi^2 e^2}{m^2 \omega^2} \rho(\omega) |\langle k | e^{i\mathbf{k}\cdot\mathbf{r}} \Delta_{A_0}' | n \rangle|^2 \qquad \dots (199)$$

For the B coefficient, we deal with the density P(v) of radiations per unit frequency range. For it we have

$$\rho(\omega) d\omega = \rho(\omega) 2\pi dv = \rho(v) dv$$

$$\Rightarrow \rho(\omega) = \rho(v)/2\pi$$

$$\frac{|a_k(t)|^2}{t} = \frac{2\pi e^2}{m^2 \omega^2} \rho(v) |\langle k | e^{i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_0}, |n\rangle|^2 \dots (200)$$

From the definition, it should be equal to $B \rho$ (v). Therefore,

$$B = \frac{2\pi e^2}{m^2 \omega^2} |\langle k | e^{i\mathbf{k}\cdot\mathbf{r}} \nabla_{A_0}, | n \rangle|^2 \qquad \dots (201)$$

For a dipole transition, this can be simplified to the expression,

$$B = \frac{2\pi c^2}{3\hbar^2} |\langle k | r | n \rangle|^2 \qquad ...(202)$$

Using it we can find out the A coefficient without going into full quantum mechanical calculations. For it we have

$$N_1 B \rho (v) = N_2 [A + B \rho (v)]$$

 $B \rho (v) = \frac{N_2}{N_1} [A + B \rho (v)]$

or

or

$$\frac{N_1}{N_2} B \rho (v) = A + B \rho (v)$$

$$\Rightarrow A = \left(\frac{N_1}{N_2} - 1\right) B \rho (v)$$

From Boltzmann distribution formula we have:

$$\frac{N_2}{N_1} = e^{-h\nu/hT}$$

$$\therefore A = (e^{h\nu/hT} - 1) B \rho(\nu)$$

Substituting the value of B from eqn. (202) and the value of ρ (v) from eqn. (155) we get

$$A = (e^{h\nu/kT} - 1) \cdot \frac{2\pi e^2}{3\hbar^2} \cdot |\langle k \mid \mathbf{r} \mid n \rangle|^2 \frac{8\pi\nu^3 h}{c^3} \frac{1}{(e^{h\nu/kT} - 1)}$$

$$= \frac{16\pi^2 \nu^3 e^2}{3c^2} \cdot \frac{h}{\hbar^2} \cdot |\langle k \mid \mathbf{r} \mid n \rangle|^2$$

$$A = \frac{4e^2\omega^3}{3\hbar c^3} |\langle k \mid \mathbf{r} \mid n \rangle^2 \dots$$

This gives the probability per unit time for spontaneous emission of a photon.

"Problems"

Problem 1. Consider a hydrogen atom in the Schroedinger theory. To what extent can the degeneracy of its first excited state be removed by a constant electric field &?

Sol. The splitting of the energy levels of an atom due to a uniform external electric field is called the Stark effect. It is due to this effect that the degenerate n=2 state of hydrogen atom will be splitted into more than one state; and in order to estimate the extent to which the degneracy is removed, we use the time independent perturbation theory for degenerate case, discussed in section. 8.2 of this chapte.

The first excited state (n=2) of hydrogen atom is four-fold degenerate. The quantum numbers l, m have the values (0, 0), (1, 0) (1, 1) and (1, -1). Hence the secular equation for the problem can be writen as in eqn. (i) on page 339: where the perturbation H' is the interaction of the electron with the electric field and it is given by $H'=eEz=eEr\cos\theta \qquad ...(ii)$

 $H'=eEz=eEr\cos\theta$...(ii) We have taken the direction of E as the z-axis. The state $|l,m\rangle$ stands for the wavefunction ψ_{2lm} of the hydrogen atom,

 $\psi_{2lm} = R_{2l} (r) \Theta_{im} \Phi_m \qquad ...(iii)$

Now it is clear that H' is odd with respect to the space inversion r, θ , $\phi \rightarrow r$, $\pi - \theta$, $\phi + \pi$). Radial wavefunction R(r) is unchanged, the Φ_m part of ψ given

 $\Phi_m = \frac{1}{\sqrt{2\pi}} e^{im\phi},$

changes the sign if m is odd and remains unchanged if m is even, and the Θ_m part given by

 $\Theta_{lm}(\theta) = \sqrt{\left(\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}\right)}P_{l}^{m}(\cos\theta);$

changes sign if (l-m) is odd and remains unchanged if (l-m) is even. Thus ψ_{2lm} changes sign (odd parity) or remains unchanged (even parity) on space inversion, depending upon whethern the quantum number l is odd or even.*

*Under the change $\phi \to \phi + \pi$, $e^{im\phi} \to e^{im(\phi + \pi)} = (-1)^m e^{im\phi}$

Thus Φ_m has the parity of m. Further, as $\theta \to \pi - \theta$, $\cos \theta \to \cos (\pi - \theta)$ $= -\cos \theta$, and $\sin \theta \to \sin \theta$. Therefore, the factor $(1 - \cos^2 \theta) \mid m \mid l^2 = \sin \mid m \mid \theta$ in P_l^m (cos θ) is unaffected, while the polynomial factor acquires a sign $(-1)^{l-|m|}$

(1, 0 | H' | 1, 1) < (0, 0 | H' | 1, 1) <($((1, 1 \mid H' \mid 1, 1) ((1, 0 \mid H' \mid 1, 0) - E_1)$ ⟨0, 0 | H' | 1, 0⟩ $\langle 1, 1 \mid H' \mid 1, 0 \rangle$

Since the perturbation H' is odd w.r.t. space inversion, the only non zero matrix elements of H' are those which correspond to the states with opposite parities. Hence the secular equation (i) reduces to

$$\begin{vmatrix}
-E_1 & \langle 0, 0 | H' | 1, 0 \rangle & 0 & 0 \\
\langle 1, 0 | H' | 0, 0 \rangle & -E_1 & 0 & 0 \\
0 & 0 & -E_1 & 0 \\
0 & 0 & -E_1 \end{vmatrix} = 0 \quad ...(iv)$$
Now

Now,

$$\langle 1, 0 \mid H' \mid 0, 0 \rangle = \langle 0, 0 \mid H' \mid 1, 0 \rangle = \int \psi_{210} H' \psi_{200} d^3r \dots (v)$$

Substituting the values of ψ_{210} , H' and ψ_{200} , we get:

$$\int \psi_{210} H' \ \psi_{200} \ d^3r = \frac{e\xi}{\sqrt{(4\pi)}} \cdot \int \left(\frac{3}{4\pi}\right) \left\{ \left[\int_0^\infty \left(\frac{1}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0} \right] \times \frac{1}{(2a_0)^{3/2}} \frac{r}{a_0 \sqrt{(3)}} e^{-r/2a_0} r^3 dr \right\} \times \left[\int_0^\pi \cos^2 \theta \sin \theta \ d\theta \right] \left[\int_0^{2\pi} d\phi \right] \right\} \dots (vi)$$

Now,
$$\int_0^{\pi} \cos^2 \theta \sin \theta \ d\theta = -\frac{1}{3} \left[\cos^3 \theta \right]_0^{\pi} = \frac{2}{3}$$
,

$$\int_0^{2\pi} d\phi = 2\pi, \text{ and}$$

$$\int_0^{\infty} \left(\frac{1}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0} \left(\frac{1}{2a_0}\right)^{3/2} \frac{1}{a_0\sqrt{3}} e^{-r/2a_0} r^4 dr$$

$$= \left(\frac{1}{2a_0}\right)^3 \frac{1}{a_0\sqrt{(3)}} \int_0^\infty \left(2 - \frac{r}{a_0}\right) e^{-r/a_0} r^4 dr$$

$$= \left(\frac{1}{2a_0}\right)^3 \frac{1}{a_0\sqrt{(3)}} \cdot \left[\frac{2.4!}{(1/a_0)^5} - \frac{1}{a_0} \cdot \frac{5!}{(1/a_0)^6}\right]$$

$$\left\{ \because \int_{0}^{\infty} e^{-\alpha r} r^n dr = \frac{n!}{a_0+1} \right\}$$

$$= \left(\frac{1}{2a_0}\right)^3 \cdot \frac{1}{a_0\sqrt{(3)}} \cdot (-72a_0^5) = -3\sqrt{(3)} \ a_0$$

Substituting these values in (vi), we have

$$\int \psi_{210} H' \psi_{200} d^3r = \frac{e\mathcal{E}}{\sqrt{(4\pi)}} \cdot \sqrt{\left(\frac{3}{4\pi}\right) \cdot \frac{2}{3}} \cdot 2\pi \cdot (-3\sqrt{3}) a_c$$

 $=-3e \xi a_0$(vii)

Using it into (iv) we write the secular equation as:

$$\begin{vmatrix}
-E_1 & -3e & \epsilon a_0 & 0 & 0 \\
-3e & \epsilon a_0 & -E_1 & 0 & 0 \\
0 & 0 & -E_1 & 0 \\
0 & 0 & 0 & -E_1
\end{vmatrix} = 0 ...(viii)$$

The four roots of (viii) are,

$$E_1 = 0, 0, +3e \& a_0 \text{ and } -3e \& a_0$$

Thus half of the fourfold degeneracy is removed in the first order. Two of the four degenerate states are unaffected by the electric field in the first order and the other two form linear combinations with extra energies $\pm 3e \mathcal{E} a_0$. The first two values of E_1 correspond to any two linearly independent combinations of ψ_{211} and ψ_{21} , -1, which has the same parity (odd.), and the third and fourth values of E_1 correspond to the linear combinations of ψ_{200} and ψ_{210} . In order to find these, let us represent them by v_1 and v_2 as:

and,
$$v_1 = a_{11} \psi_{200} + a_{21} \psi_{210}$$
 and, $v_2 = a_{21} \psi_{200} + a_{22} \psi_{200}$ \cdots (x)
Let $H' v_1 = 3e \mathcal{E} a_0 v_1$ and $H' v_2 = -3e \mathcal{E} a_0 v_2$ \cdots (xi)

Eqns. (xi) can be written in matrix form as:

$$\binom{0}{3e\&a_0} \binom{3e\&a_0}{0} \binom{a_{11}}{a_{21}} = 3e\&a_0 \binom{a_{11}}{a_{21}} \text{ and } \binom{0}{3e\&a_0} \binom{3e\&a_0}{0} \binom{a_{21}}{a_{22}}$$

$$= -3e\&a_0 \binom{a_{21}}{a_{22}}$$

To satisfy these equations,

$$a_{21} = a_{11}$$
 and $a_{22} = -a_{21}$...(xii)

 $v_1 = a_{11}(\psi_{200} + \psi_{210}) \text{ and } v_2 = a_{22}(\psi_{200} - \psi_{210})$

Normalizing v_1 and v_2 we have,

$$v_1 = \frac{1}{\sqrt{(2)}} (\psi_{200} + \psi_{210}) \text{ and } v_2 = \frac{1}{\sqrt{(2)}} (\psi_{200} - \psi_{210}) \dots (xiii)$$

This means that a hydrogen atom in its first excited state behaves as though it has a permanent electric dipole moment of magnitude 3eao that can be oriented in three different ways: one state parallel to the external field, one state antiparallel to the field and two states with zero components along the field.

First order splitting of energy levels.

Problem 2. Derive an expression for the shift in ground state energy level of the hydrogen atom due to a weak external electric field to order &2, where & is the magnitude of the electric field.

Explain why the first order shift in the energy levels vanishes only in the ground state and not in the excited states.

Sol. The perturbation H' due to a weak uniform electric field & applied along the z-axis is given by: ...(i)

The energy of the system in the mth state under the perturbation H' to second order is given by the general formula,

$$E = E_m^{(0)} + \langle m \mid H' \mid m \rangle + \sum_{n}' \frac{\langle m \mid H' \mid n \rangle|^2}{\left(E_m^{(0)} - E_n^{(0)}\right)} \dots (ii)$$

In the present case $E_m^{(0)}$ is the ground state energy of hydrogen atom and m is the ground state, ψ_{100} , of the hydrogen atom. Therefore, expression (ii) for the ground state of hydrogen can be written as:

written as .
$$E = \frac{-e^2}{2a_0} + \langle 0 \mid H' \mid 0 \rangle + \sum_{n \neq 0} \frac{|\langle 0 \mid H' \mid n \rangle|^2}{(E_0 - E_n)}, \dots (iii)$$

where $E_0 = -\frac{e^2}{2a_0}$ is the ground state energy of hydrogen atom and we designate the ground state by | 0>.

Now, $\langle 0 \mid H' \mid 0 \rangle$ vanishes, because the nondegenerate ground state ψ_{100} has even parity. Hence we have

$$E = \frac{-e^2}{2a_0} + e^2 \mathcal{E}^2 \sum \frac{|\langle 0 | z | n \rangle|^2}{(E_0 - E_n)} \qquad ...(iv)$$

$$E = \frac{-e^2}{2a_0} + e^2 \mathcal{E}^2 \sum \frac{|\langle 0 | z | n \rangle|^2}{(E_0 - E_n)} \qquad ...(iv)$$

In order to evaluate the second term in eqn. (iv) we apply the following technique:

Suppose that we can find an operator F which satisfies the equation

...(v) $z\mid 0\rangle = (FH_0 - H_0F)\mid 0\rangle,$

where H_0 is the unperturbed Hamiltonian of hydrogen atom. Then we have,

we have,

$$\langle n \mid z \mid 0 \rangle = \langle n \mid FH_0 \mid 0 \rangle - \langle n \mid H_0 F \mid 0 \rangle$$

$$= \langle E_0 - E_n \rangle \langle n \mid F \mid 0 \rangle$$
...(vi)

and,

$$\sum_{n \neq 0} \frac{|\langle 0 \mid z \mid n \rangle|^{2}}{(E_{0} - E_{n})} = \sum_{n \neq 0} \langle 0 \mid z \mid n \rangle \langle n \mid F \mid 0 \rangle$$

$$= \langle 0 \mid zF \mid 0 \rangle - \langle 0 \mid z \mid 0 \rangle \langle 0 \mid F \mid 0 \rangle \qquad \dots \text{(vii)}$$

Now H_0 is given by,

$$H_{0} = -\frac{\hbar^{2}}{2\mu} \nabla^{2} - \frac{e^{2}}{r} = \frac{-\hbar^{2}}{2\mu} \left\{ \frac{1}{r^{2}} \frac{\partial}{\partial r} \left(r^{2} \frac{\partial}{\partial r} \right) + \frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^{2} \sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} \right\} - \frac{e^{2}}{r}.$$

For finding F we substitute this H_0 into (v) to get,

$$\frac{\hbar^{2}}{2\mu} \left\{ \frac{1}{r^{2}} \frac{\partial}{\partial r} \left(r^{2} \frac{\partial}{\partial r} \right) + \frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^{2} \sin^{2} \theta} \frac{\partial}{\partial \phi^{2}} \right\} F$$

$$+ \frac{e^{2}}{r} F - \frac{e^{2}}{2a_{0}} F = z$$

The solution of this differential equation can be found by the separation of variables method, we get

$$F = -\frac{\mu a_0}{\hbar^2} \left(\frac{r}{2} + a_0\right) z \qquad \dots \text{(viii)}$$

Since z is an odd operator, its expectation value, $\langle 0 \mid z \mid 0 \rangle$, w.r.t. the ground state of even parity vanishes. Thus it follows from (vii) that

$$\sum_{n \neq 0} \frac{|\langle 0 \mid z \mid n \rangle|^2}{(E_0 - E_n)} = -\frac{\mu a_0}{\hbar^2} \langle 0 \mid \left(\frac{r}{2} + a_0\right) z^2 \mid 0 \rangle \dots (ix)$$

Since the ground state of hydrogen is spherically symmetric, we have

$$\langle 0 \mid x^2 \mid 0 \rangle = \langle 0 \mid y^2 \mid 0 \rangle = \langle 0 \mid z^2 \mid 0 \rangle = \frac{1}{3} \langle 0 \mid r^2 \mid 0 \rangle$$

Hence,

$$\sum_{n\neq 0} \frac{|\langle 0 \mid z \mid n \rangle|^2}{(E_0 - E_n)} = -\frac{\mu a_0}{3\hbar^3} \left[\frac{1}{2} \langle 0 \mid r^3 \mid 0 \rangle + a_0 \langle 0 \mid r^2 \mid 0 \rangle \right] ...(x)$$

Now,

$$\langle 0 \mid r^{n} \mid 0 \rangle = \frac{1}{\pi a_{0}^{3}} \int_{0}^{e^{-2r/a_{0}}} r^{n+2} \sin \theta \, d\theta \, d\phi \, dr$$

$$= \frac{4\pi}{\pi a_{0}^{3}} \int_{0}^{\infty} e^{-2r/a_{0}} r^{n+2} \, dr$$

$$= \frac{4\pi}{\pi a_{0}^{3}} \cdot \frac{(n+2)!}{(2/a_{0})^{n+3}} \cdot \left\{ \because \int_{0}^{\infty} e^{-a_{r}} r^{n} \, dr = \frac{n!}{\alpha^{n+1}} \right\}$$

$$= \frac{a_{0}^{n} (n+2)!}{2^{n+1}}$$

Using it into (x) we finally obtain,

$$\sum_{n\neq 0}^{\frac{1}{(0|z|n)^2}} \frac{|a_0|}{(E_0 - E_n)} = -\frac{\mu a_0}{3\hbar^2} \left[\frac{1}{2} \cdot \frac{a_0^3 \cdot 5!}{2^4} + a_0 \cdot \frac{a_0^2 \cdot 4!}{2^3} \right] = -\frac{9}{4} \frac{\mu a_0^4}{\hbar^2}.$$

$$E = -\frac{e^2}{2a_0} - e^2 \xi^2 \cdot \frac{9}{4} \frac{\mu a_0^4}{\hbar^2}$$

$$= \frac{-e^2}{2a_0} - e^2 \mathcal{E}^2 \cdot \frac{9}{4} \frac{\mu a_0^3}{\hbar^2} \cdot \frac{\hbar^2}{\mu e^2} \quad \left\{ \because \quad a_0 = \frac{\hbar^2}{\hbar e^2} \right\}$$

$$= -\frac{e^2}{2a_0} - \frac{9}{4} a_0^3 \mathcal{E}^2. \quad \dots \text{(xii)}$$

The first order shift corresponds to the matrix element $\langle 0 \mid H' \mid 0 \rangle$ which vanishes because $\mid 0 \rangle$ has a definite parity (even). While the excited states of hydrogen are degenerate and the first order matrix elements between the combination of states with different parities does not vanish and such combination of states is available for every excited state of hydrogen atom. As an example, the first excited state is considered in the previous problem.

Problem 3. An atom is placed in a uniform weak magnetic field of strength **H**. Treating the interaction between the atom and the field as a small perturbation, calculate the change in the energy levels of the atom due to this interaction.

Sol. The change in the energy levels of an atom when it is placed in a uniform external magnetic field is called the Zeeman effect. The unperturbed Hamiltonian for an electron in the atom can be written as

$$H_0 = \frac{p^2}{2m} - \frac{Ze^2}{r},$$
 ...(i)

where Z is the number of protons in the nucleus. We know that the effect of the magnetic field on the orbital motion is taken into account with the replacement $p \rightarrow p - \frac{eA}{c}$, where A is the vector potential of the field, and it is given by

$$H = \nabla \times A$$
 or $A = \frac{1}{2} (H \times r)$.

Hence the new Hamiltonian for the electron is given by

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e\mathbf{A}}{c} \right)^2 - \frac{Ze^2}{r}$$

$$= \frac{p^2}{2m} - \frac{e}{2mc} \left(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p} \right) + \frac{e^2}{2mc^2} A^2 - \frac{Ze^2}{r}$$

$$= \left(\frac{p^2}{2m} - \frac{Ze^2}{r} \right) - \frac{e}{mc} \mathbf{A} \cdot \mathbf{p}.$$
(ii)

Now, $A \cdot p = \frac{1}{2} (H \times r) \cdot p = \frac{1}{2} H \cdot (r \times p) = \frac{1}{2} H \cdot L$, where L is the orbital angular momentum of the electron. Thus

$$H = H_0 - \frac{e}{2mc} + \mathbf{H} \cdot \mathbf{L} + \frac{e^2}{2mc^2} A^2$$
.

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For the first order calculations, the last term in the above, which is quadratic in H, can be neglected. Hence we have

The second term on the right hand side of (iii) is the interaction of H with the orbital motion and it has the form of the interaction energy of H with a magnetic moment given by

$$\mu_L = \frac{e}{2mc} L. \qquad ...(iv)$$

This is the magnetic moment associated with the orbital motion.

Similarly, the energy of interaction of the spin magnetic mo-

ment μ_s with H is given by $-\mu_s$ oH, where

$$\overrightarrow{\mu_S} = \frac{e}{mc} S \qquad \dots (v)$$

Note that the gyromagnetic ratio (e/mc) associated with spin imption has double the value of the ratio in the case of orbital imption. This was first deduced empirically (from atomic spectra), but comes out as an automatic consequence of the Dirac's relativistic theory.

Therefore, including the interaction of H with spin magnetic. imoment, we get the Hamiltonian

$$H = H_0 - \frac{e^{\frac{1}{16}}}{2mc} \cdot (L + 2S).$$
 ...(vi)

The spin magnetic moment μ_S can also interact with the imagnetic field created by its orbital motion. The energy associated with this spin-orbit interaction is proportional to L.S. When the electron is in a potential V(r), assumed to be spherically symmetric, the proportionality factor can be shown to be

$$(2m^2c^2r)^{-1}(dV/dr)$$
.

Thus the so called spin orbit energy gives a contribution,

$$\frac{1}{2m^2c^2}\cdot\frac{1}{r}\frac{dV}{dr},$$
 ...(vii)

rate atomic levels, thereby giving rise to the fine structure in atomic spectra. In the non-relativistic case we can neglect this interaction. Therefore, neglecting spin-orbit interaction, the perturbation part of the Hamiltonian which gives rise to Zeeman ceffect is given by

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$$H' = -\frac{eH}{2mc} \cdot (\mathbf{L} + 2\mathbf{S}) = -\frac{eH}{2mc} \cdot (\mathbf{J} + \mathbf{S}). \tag{viii}$$

The eigenstates of the unperturbed Hamiltonian H_0 are the simultaneous eigenstates of the operators L^2 , S^2 and J^2 ; because all of these operators commute with H_0 . Hence the unperturbed states can be denoted by $| lsjm \rangle$, and the change in the energy in the first order is given by

$$\triangle E = \langle lsjm \mid H' \mid lsjm \rangle. \qquad ...(ix)$$

Now we have,

$$\langle lsjm \mid S \mid lsjm \rangle = \langle lsjm \mid \frac{J \cdot S}{j(j+1) \hbar^2} J \mid lsjm \rangle$$

and from

$$J-S=L$$
,
 $J \cdot S=\frac{1}{2} (J^2+S^2-L^2)$.

we have

$$\therefore \langle lsjm \mid \mathbf{S} \mid lsjm \rangle = \langle m \mid \mathbf{J} \mid m \rangle. \frac{j(j+1)+s(s+1)-l(l+1)}{2j(j+1)}$$

Hence we get from eqns. (ix) and (viii),

$$\Delta E = \frac{-e}{2mc} \langle m \mid \overrightarrow{H} \cdot \mathbf{J} \mid m \rangle \left\{ 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \right\}$$

or

$$\triangle E = -\frac{e}{2mc} + \ln m_j g \qquad ...(x)$$

provided that the axis of the quantization is taken in the direction of H. The factor

$$g=1+\frac{j(j+1)+s(s+1)-l(l+1)}{2j(j+1)}$$
...(xi)

is the Lande splitting factor, which was constructed from empirical analysis of Zeeman spectra before the advent of quantum mechanics.

The magnetic quantum number m_j has (2j+1) values as j, j-1, ..., -j. Thus the unperturbed level is splitted into (2j+1) levels with constant spacing $\frac{e\hbar g}{2mc}$ H. Some typical values of g are: g=2 for ${}^2S_{1/2}$, $g=\frac{2}{3}$ for ${}^2P_{1/2}$, $g=\frac{4}{3}$ for ${}^2P_{3/2}$ etc.

Problem 4. How do the D_1 and D_2 lines of sodium split in the presence of an external magnetic field of strength H.

Sol. The D_1 and D_2 lines correspond to the transitions $P_{1/2} \rightarrow S_{1/2}$ and $P_{3/2} \rightarrow S_{1/2}$; respectively. Thus, there are three terms: $P_{3/2}$, $P_{1/2}$ and $S_{1/2}$. From eqn. (x) it is clear that the splitting of these terms in the presence of the external magnetic

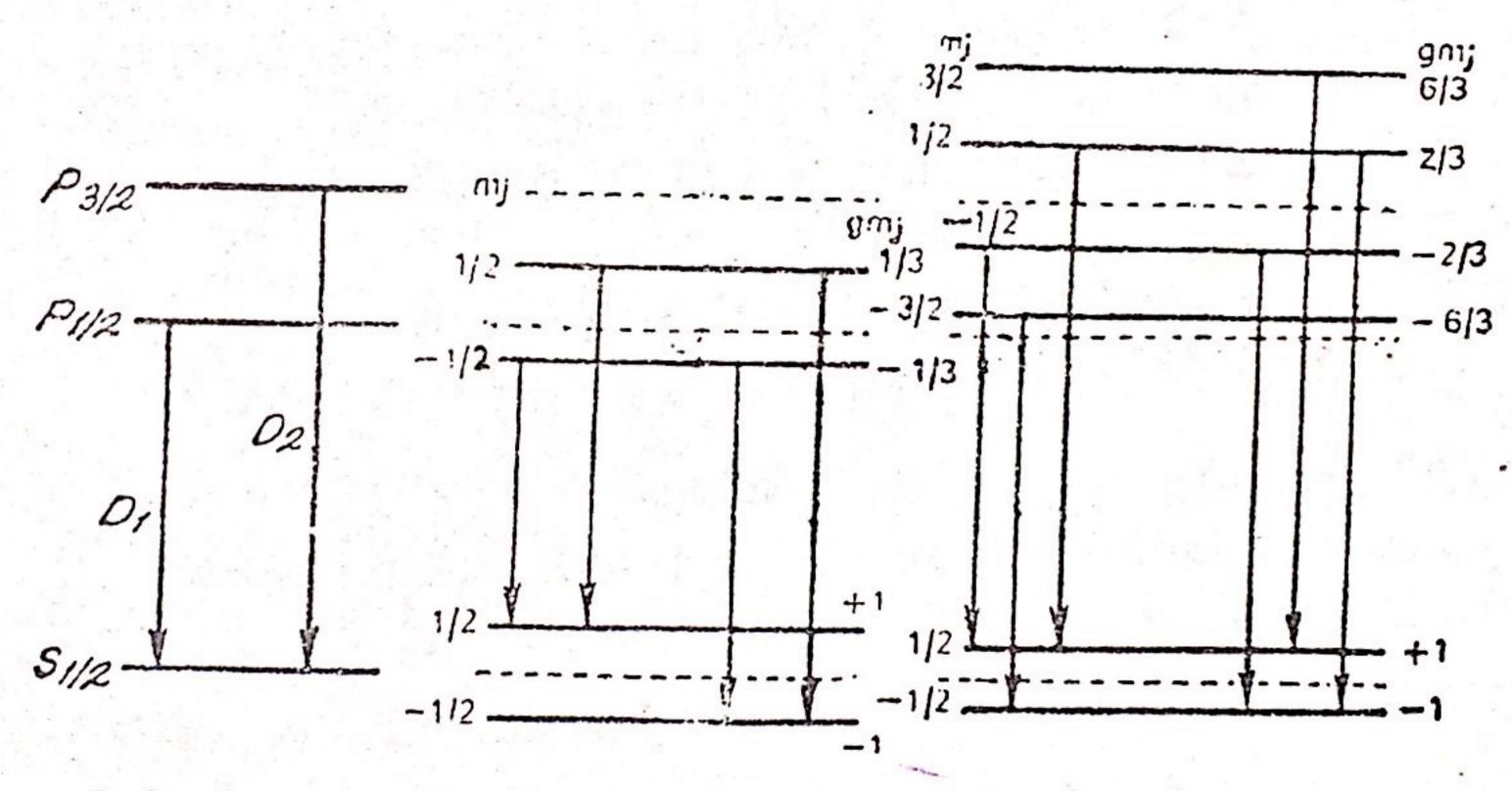
field H depends on the factor gm_j . So we calculate this factor for all the three terms. For $P_{3/2}$ state, l=1, $s=\frac{1}{2}$ and $j=\frac{3}{2}$.

$$\therefore g = 1 + \frac{\frac{3}{2} \left(\frac{3}{2} + 1\right) + \frac{3}{4} - 1 \cdot (1 + 1)}{2 \cdot \frac{3}{2} \left(\frac{3}{2} + 1\right)} = \frac{4}{3}.$$

Now m_j can have four values; $\frac{3}{2}$, $\frac{1}{2}$, $-\frac{1}{2}$ and $-\frac{3}{2}$. Hence gm_j has the values: 2, $\frac{2}{3}$, $-\frac{2}{3}$ and -2. Similarly, the splitting factor can be calculated for the other two terms, and all of these are listed below:

Terms	1	S	\boldsymbol{j}	gm_1
$P_{3/2}$	1	$\frac{1}{2}$	32	$2, \frac{2}{3}, -\frac{2}{3}, -2$
$P_{1/2}$	1 :	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{3}, -\frac{1}{3}$
$S_{1/2}$	0	$\frac{1}{2}$	1 2	1, -1.

The possible transitions for the splitted D_1 and D_2 levels are illustrated below. The selection rules are $\Delta m_j = 0$, ± 1 and $\Delta j = \pm 1$.



It is clear that D_1 line splits into four, while D_2 into six components; symmetrically situated about the normal positions.

Problem 5. The spin-orbit interaction introduces a term in the Hamiltonian of the form

$$H'=\xi(r) \mathbf{L} \cdot \mathbf{S}$$

where $\xi(r)=(1/2m^2c^2)[(1/r)(dV/dr)]$ for the motion of the electron through the static electric field of potential V(r). Show that the energies of the perturbed states are

$$E=E_0+\left\{\begin{array}{ll} \frac{1}{2}l\zeta_{nl}, & j=l+\frac{1}{2}\\ -\frac{1}{2}(l+1)\zeta_{nl}, & j=l-\frac{1}{2}, \end{array}\right.$$

$$\zeta_{nl} = \hbar^2 \int_0^\infty R_{nl}^2 (r) \xi (r) r^2 dr,$$

and Eo is the energy of the unperturbed level.

Sol. If H_0 is the unperturbed Hamiltonian, then the total Hamiltonian including spin-orbit interaction can be written as $H=H_0+H'$; $H=\xi(r)$ L·S is the perturbation part.

The states of an electron in the unpertubred atom can be written in the form

$$\psi = R_{n_l}(r) Y_1^{m_l}(\theta, \phi) \chi(m_s),$$

where R is the radial part. $Y_i^{m_l}$ is the angular and χ the spin part of the wavefunction.

From the first order perturbation theory, change in the unperturbed energy E_0 due to the perturbation H' is given by

$$\langle \psi \mid H' \mid \psi \rangle = \langle \psi \mid \xi (r) \text{ L·S} \mid \psi \rangle.$$
 ...(i)

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Now J=L+S gives

$$J^2 = L^2 + S^2 + 2L \cdot S$$

 $L \cdot S = (J^2 - L^2 - S^2)/2$.

or

Since $s=\frac{1}{2}$ for the electron and hence j can be either $l+\frac{1}{2}$ or $l-\frac{1}{2}$. Therefore,

$$\langle \psi \mid \mathbf{L} \cdot \mathbf{S} \mid \psi \rangle = \frac{1}{2} \left[(l + \frac{1}{2}) (l + \frac{3}{2}) - l (l + 1) - \frac{1}{2} (\frac{1}{2} + 1) \right] \hbar^{2}$$

$$= \frac{1}{2} l \hbar^{2} \quad \text{for } j = l + \frac{1}{2}$$
 ...(ii)

and

 $\langle \psi \mid \mathbf{L} \cdot \mathbf{S} \mid \psi \rangle = -\frac{1}{2} (l+1) \, \hbar^2$ for $j = l - \frac{1}{2}$(iii) Using (ii) and (iii) into (i) we get the first order perturbation arising from ξ (r) $\mathbf{L} \cdot \mathbf{S}$ as:

$$\langle \psi | H' | \psi \rangle = \left\{ \int R_{nl}^* (r) Y_l^{m_l^*} (\theta, \phi) \chi^* (m_s) \xi(r) R_{nl}(r) Y_l^{m_l} (\theta, \phi) \right.$$

$$\chi(m_s) d^3r \right\} \times \left\{ \frac{1}{2} l \hbar^2 ; j = l + \frac{1}{2} \right.$$

$$\left. - \frac{1}{2} (l+1) \hbar^2 ; j = l - \frac{1}{2} \right.$$

Using the normality of $Y_l^{m_l}$ and χ (m_s) we can write,

Therefore, the energy of the perturbed state is given by: $E = E_0 + \langle \psi \mid H' \mid \psi \rangle$

$$=E_{0}+\begin{cases} \frac{1}{2}l\zeta_{nl} & ; j=l+\frac{1}{2}\\ -\frac{1}{2}(l+1)\zeta_{nl} & ; j=l-\frac{1}{2} \end{cases}$$
Where, $\zeta_{nl}=\hbar^{2}\int_{0}^{\infty}R_{nl}^{2}(r)\xi(r)r^{2}dr$...(v)

Problem 6. Calculate the quantity ζ_{n1} , defined in the preceding problem, for the potential function $V(r) = -Ze^2/r$.

Sol. For the given potential function we have,

$$\xi(r) = \frac{1}{2m^2c^2} \cdot \frac{1}{r} \cdot \frac{\partial V}{\partial r} = \frac{ze^2}{2m^2c^2} \cdot \frac{1}{r^3} \qquad ...(i)$$

The radial wavefunction $R_{nl}(r)$ for an electron moving in the potential $-Ze^2/r$ is the radial part of the wavefunction for a hydrogen like atom with z-protons in the nucleus, and it is given by;

with
$$R_{nl}(r) = -\left\{ \left(\frac{2z}{na_0} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} \exp \left[-\rho/2 \right] \rho^i L_{n+l}^{2l+1}(\rho) \dots \text{(ii)}$$

$$\rho = \frac{2z}{na_0} r \dots \text{(iii)}$$

and $L_{n+l}^{2l+1}(\rho)$ is the laguerre polynomial.

Using (i), (ii) and (iii) we have,

$$\zeta_{nl} = \hbar^{2} \left(\frac{2z}{na_{0}} \right)^{3} \cdot \frac{(n-l-1)!}{2n[(n+l)!]^{3}} \cdot \frac{ze^{2}}{2m^{2}c^{2}} \times \int_{0}^{\infty} \exp(-\rho) \rho^{(2l-1)} \left[L_{n+l}^{2l+1}(\rho) \right]^{2} d\rho \qquad ...(iv)$$

To evalute the integral in (iv), we use the recurrence formula

$$(k+1) L_{k+1}^{\alpha} - (2k+\alpha+1-\rho) L_{k}^{\alpha} + (k+\alpha) L_{k-1}^{\alpha} = 0 \qquad \dots (v)$$

and the orthonormality relation for the Laguerre polynomial,

$$\int_{0}^{\omega} \exp \left(-\rho\right) \rho^{\alpha} L_{k}^{\alpha}(\rho) L_{k'}^{\alpha}(\rho)$$

$$= \begin{cases} \Gamma(\alpha+1)^{k+\alpha} \cdot C_{k} & \text{for } k=k' \\ 0 & \text{for } k\neq k' \end{cases} \dots \text{(vi)}$$

From (v) we have,

$$\rho L_{k}^{\alpha} = (2k + \alpha + 1) L_{k}^{\alpha} - (k+1)L_{k+1}^{\alpha} - (k+\alpha)L_{k-1}^{\alpha} \dots (vii)$$

Multiplying (vii) by

$$e^{-\rho} \, \mathcal{F}^{\alpha-1} L_k^{\alpha}$$

and integrating we obtain, using (vi), as

$$\int_{0}^{\infty} e^{-\rho \rho \alpha} \left[L_{k}^{\alpha} \right]^{2} d\rho = (2k + \alpha + 1) \int_{0}^{\infty} e^{-\rho \rho \alpha - 1} \left[L_{k}^{\alpha} \right]^{2} d\rho$$
or
$$\int_{0}^{\infty} e^{-\rho \rho \alpha - 1} \left[L_{k}^{\alpha} \right]^{2} d\rho = \frac{1}{(2k + \alpha + 1)} \cdot \Gamma(\alpha + 1)^{k + \alpha} C_{k} \dots \text{(viii)}$$
Again, multiplying (vii) by

$$e^{-\rho} \rho^{\alpha-2} L_{l}^{\alpha}$$

and integrating we obtain, using (vi) and (viii), as

$$\int_{0}^{\infty} e^{-\rho} \rho^{\alpha-2} \left[L_{k}^{\alpha} \right]^{2} d\rho = \frac{1}{(2k+\alpha+1)^{2}} \cdot \Gamma(\alpha+1)^{k+\alpha} C_{k} \qquad \dots (ix)$$

Taking $\alpha = 2l+1$ and k=n+l we get from (ix) as

$$\int_{0}^{\infty} e^{-\rho} \rho^{(2l-1)} \left[L_{n+l}^{2l+1} \right]^{2} d\rho = \frac{1}{(2n+4l+2)^{2}}.$$

$$\Gamma(2l+2)^{n+3l+1} C_{n+l} \dots(x)$$

Using it into (iv) and making some algebraic simplifications we obtain

$$\zeta_{nl} = \frac{e \, \hbar^2}{2m^2c^2a_0^3} \cdot \frac{z^4}{n^3l(l+\frac{1}{2})(l+1)} \cdot \dots (xi)$$

Problem 7. If a particle is scattered by a weak potential V(r); calculate the differential scattering cross section by treating the interaction between the free-particle state and the potential V(r) as a small perturbation.

Sol. Let us denote the initial and the final states of the free particle by the plane waves,

 $\psi_i = L^{-3/2} \exp$. $(i\mathbf{k}_0 \cdot \mathbf{r})$ and $\psi_f = L^{-3/2} \exp$. $(i\mathbf{k} \cdot \mathbf{r})$...(i) where \mathbf{k}_0 and \mathbf{k} are the initial and the final propagation vectors; respectively, and the wavefunctions are normalized over a cubical box of side L.

Since the potential V(r) is independent of time, the transition probability per unit time from the initial state ψ_i to the final state ψ_i is given by the formula

$$w = \frac{2\pi}{\hbar} \rho(k) |H'|_{fi}|^2; \qquad \dots (ii)$$

where $\rho(k)$ is the density of the final states, and the perturbation matrix element H'_{fi} is given by

$$H'_{fi} = \int \psi^*_f H' \psi_i d^3r$$

$$= \int \frac{1}{L^{3/2}} \exp[-i\mathbf{k} \cdot \mathbf{r}] V(r) \frac{1}{L^{3/2}} \exp[i\mathbf{k}_0 \cdot \mathbf{r}] d^3r$$

$$= \frac{1}{L^3} \int \exp \left[i(\mathbf{k}_0 - \mathbf{k}) \cdot r\right] V(r) d^3r$$

$$|H'|_{ft}|^2 = \frac{1}{L^6} \left| \int \exp \left[i(\mathbf{k}_0 - \mathbf{k}) \cdot r\right] V(r) d^3r \right|^2 \dots (iii)$$

The value of $\rho(k)$ can be calculated as follows:

For the case of a cubical box of length L, the normalized wavefunctions and eigen-values are given by

$$\psi_{n_{x}n_{y}n_{z}} = \frac{1}{(L/2)^{3}} \sin \frac{n_{x}\pi x}{L} \sin \frac{n_{y}\pi y}{L} \sin \frac{n_{z}\pi z}{L}$$
and
$$E = \frac{\hbar^{2}\pi^{2}}{2m L^{2}} n^{2}, \text{ where } n^{2} = n_{x}^{2} + n_{y}^{2} + n_{z}^{2}.$$
or
$$\frac{\hbar^{2}k^{2}}{2m} = \frac{\hbar^{2}\pi^{2}}{2mL^{2}} n^{2}$$

$$\Rightarrow k_{x}^{2} = \frac{\pi^{2}n_{x}^{2}}{L^{2}}, k_{y}^{2} = \frac{\pi^{2}n_{y}^{2}}{L^{2}}, k_{z}^{2} = \frac{\pi^{2}n_{z}^{2}}{L^{2}}$$

$$\therefore k_{x} = \pm \frac{\pi n_{x}}{L}; k_{y} = \pm \frac{\pi n_{y}}{L} \text{ and } k_{z} = \pm \frac{\pi n_{z}}{L} \qquad ... \text{(iv)}$$

The permitted values of k in the box are, therefore, given by

$$k_x = \frac{2\pi n_x}{L}$$
, $k_y = \frac{2\pi n_y}{L}$, $k_z = \frac{2\pi n_z}{L}$

where, n_x , n_y , n_z are positive or negative integers or zero. Hence the volume occupied by one state in the k-space will be $\left(\frac{2\pi}{L}\right)^3$, and the number of states in the volume element $d^3k = k^2dk \sin\theta \ d\theta$ will be given by

$$\left(\frac{L}{2\pi}\right)^3 k^2 dk \sin\theta \, d\theta \, d\phi$$

or

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$$\frac{m}{\hbar^2} \left(\frac{L}{2\pi}\right)^3 k \ dE_k d\Omega$$

$$\left\{ : E_{k} = \frac{\hbar^{2} k^{2}}{2m} \Rightarrow k dk = \frac{m}{\hbar^{2}} dE_{k} \right\}$$

.. Number of final states per unit energy range is given by

$$\rho(k) = \frac{mL^3}{8\pi^3 \hbar^2} \cdot k \cdot d\Omega \qquad \dots (v)$$

Substituting (iii) and (v) into (ii), we get the probability per unit time for a transition to a final state in solid angle $d\Omega$ as:

$$w = \frac{2\pi}{\hbar} \frac{mL^3}{\hbar^2} \cdot k. \frac{1}{L^6} \left| \int \exp \left[ik_0 - k \right) \cdot r \right] V(r) d^3 r \left|^2 \frac{d\Omega}{8\pi^3} \right|^2$$

$$= \frac{2\pi m}{\hbar^3 L^3} k \left| \int \exp \left[i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r} \right] V(r) d^3 r \right|^2 \frac{d\Omega}{8\pi^3} \dots (vi)$$

This is equal to the number of particles scattered into the solid angle element $d\Omega$ per unit time, when there is one incident particle in the volume L^3 . If there are N particles incident with velocity v within a unit volume, then the incident flux (number of particles crossing a unit area of cross-section per unit time time) is equal to Nv.

Since the velocity of the incident particles is $\frac{p_0}{m} = \frac{\hbar k_0}{m}$; the incident flux is therefore, given by

$$S_i = \frac{v}{L^3} = \frac{\hbar k_0}{mL^3}$$

 $\left(\begin{array}{c} \cdot \cdot \frac{1}{L^3} \end{array}\right)$ is the number of incident particles per unit volume.

If N_s is the number of particles scattered in the solid angle $d\Omega$ per second, then the differential scattering cross-section $(d\sigma/d\Omega)$ is defined by

$$N_s = S_i \left(\frac{d\sigma}{d\Omega}\right) . d\Omega$$
 ...(vii)

Now N_s is equal to was described above, therefore,

$$\frac{2\pi m}{\hbar^3 L^3} k \left| \int e^{i (k_0 - k) \cdot r} V(r) d^3 r \right|^2 \frac{d\Omega}{8\pi^3} = \frac{\hbar k_0}{mL^3} \left(\frac{d\sigma}{d\Omega} \right) d\Omega. \quad ... \text{(viii)}$$

For elastic scattering, in which the energy of the initial particle remains unchanged after scattering, $k_0 = k$. Therefore

$$\left(\frac{d\sigma}{d\Omega}\right) = \left|\frac{1}{4\pi} \cdot \frac{2m}{n^2}\right| e^{i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}} V(r) d^3r. \quad |^2 \dots (ix)$$

It will be seen in the theory of Scattering that the Born approximation (equation 170 of chapter-9) gives exactly the same result as obtained here from the pertubration theory.

Problem 8. Use the time dependent perturbition theory for harmonic perturbation to calculate the ionization probability of a kydrogen atom from its ground state

$$\psi_{100} = \frac{1}{\sqrt{(\pi a_0^3)}} e^{-r/a_0}, \qquad \dots (i)$$

where a_0 is the first Bohr's radius. Would the threshold energy regired io ionize the atom from the stae ψ_{200} be more or less?

Sol. For the ionization of the hydrogen atom intially in its ground state, we place it in a harmonically time-varying electric

field

 $\mathbf{E}(t) = 2\mathbf{E}_0 \sin \omega t$.

The interaction of this field with the electron in the ground state of hydrogen atom is given by

 $H'=e\mathbf{E}(t)\cdot\mathbf{r}=eE(t)r\cos\theta''=2eE_0r\cos\theta''\sin\omega t$ where ${\bf r}$ is the position vector of the electron and ${\boldsymbol \theta}''$ is the angle between the electric field E (t) and r.

The initial state is the ψ_{100} state of hydrogen

$$\psi_n = \frac{1}{\sqrt{(\pi a_0^3)}} e^{-r/a_0}.$$
 (iv)

The final state is the free-electron after ionization has occured. Hence the final state can be represented by the plane wave

$$\psi_k = L^{-3/2} e^{i\mathbf{k} \cdot \mathbf{r}},$$
 ...(v)

where k is the propagation vector of the ejected electron.

Now the probability of ionization can be caclulated by using the formula for the harmonic perturbation,

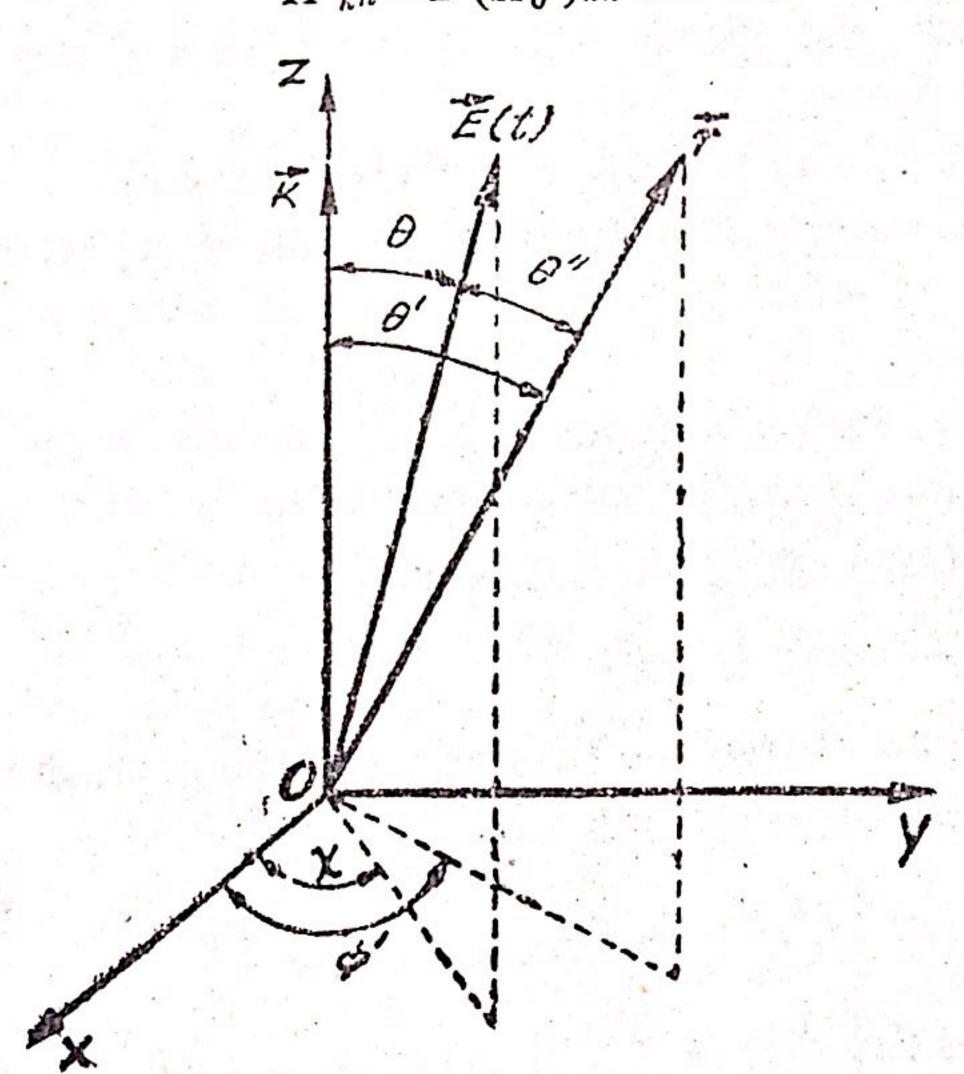
$$w = \frac{2\pi}{\hbar} \rho(k) |(H_0')_{kn}|^2, ...(vi)$$

where $\rho(k)$ is the density of the final states and it is given by eqn. (v) of the last problem,

$$\rho(k) = \frac{mL^3}{8\pi^3\hbar^2} k d\Omega$$
 ... (vii)

The matrix element $(H_0)_{kn}$ is given by

$$H'_{kn}=2 (H_0')_{kn} \sin \omega t. \qquad(viii)$$



Using equation (iii), we find that $(H_0')_{kn} = (eE_0r \cos \theta'')_{kn}$ $(E_0')_{kn} = (E_0'')_{kn} = (E_0'')_{kn}$

$$=eE_0 (\pi a_0^3 L^3)^{-1/2} \int e^{-i\mathbf{k} \cdot \mathbf{r}} r \cos \theta'' e^{-r/a_0} d^3r$$

or
$$(H_0')_{kn} = eE_0 (\pi a_0^3 L^3)^{-1/2} e^{-ikr\cos\theta'} r\cos\theta' e^{-r/a_0}$$

$$\times r^2 dr d (\cos \theta') d\phi'$$
(ix)

We have chosen the direction of vector \mathbf{k} as z-axis, and θ' is the angle between \mathbf{k} and \mathbf{r} . In order to evaluate the integral in (ix), we should express θ'' in terms of θ' and θ . For it we have

$$\mathbf{E}.\mathbf{r} = (E_x r_x + E_y r_y + E_z r_z) = Er \cos \theta''$$
.

Now

 $E_x = E \sin \theta \cos \chi$, $E_y = E \sin \theta \sin \chi$ and $E_z = E \cos \theta$; $r_x = r \sin \theta' \cos \phi'$, $r_y = r \sin \theta' \sin \phi'$ and $r_z = r \cos \theta'$. $\cos \theta'' = \sin \theta \sin \theta' \cos \chi \cos \phi' + \sin \theta \sin \theta' \sin \chi \sin \phi'$.

$$+\cos\theta\cos\theta'$$

$$= \sin \theta \sin \theta' \cos (\chi - \phi') + \cos \theta \cos \theta'. \qquad ...(x)$$

The first term in the right-hand side of (x) gives no contribution to the integral (ix), because

$$\int_0^{2\pi} \cos\left(\chi - \phi'\right) d\phi' = 0.$$

Hence we can write (ix) as

$$(H_0')_{kn} = eE_0 (\pi a_0^3 L^3)^{-1/2} \cos \theta \int_0^\infty \int_{-1}^{+1} \int_0^{2\pi} e^{-i\mathbf{k}r \cos \theta'} e^{-r/a_0} \times r^3 dr \cos \theta' d (\cos \theta') d\phi$$

$$= \frac{2\pi e E_0 \cos \theta}{\sqrt{(\pi a_0^3 L^3)}} \int_0^{\infty} \int_{-1}^{+1} e^{-ikr \cos \theta'} e^{-r/a_0}$$

$$\times r^3 dr \cos \theta' d (\cos \theta')$$

Carrying out the θ' integral by parts, we obtain

$$(H_0')_{kn} = \frac{2\pi e E_0 \cos \theta}{\sqrt{(\pi a_0^8 L^8)}} \times \left[\frac{1}{k^2} \int_0^\infty \exp \left\{ -r \left(\frac{1}{a_0} + ik \right) \right\} r \, dr \right]$$

$$-\frac{1}{ik} \int_0^\infty \exp \left\{ -r \left(\frac{1}{a_0} - ik \right) \right\} r^2 \, dr$$

$$-\frac{1}{k^2} \int_0^\infty \exp \left\{ -r \left(\frac{1}{a_0} - ik \right) \right\} r \, dr$$

$$-\frac{1}{ik} \int_0^\infty \exp \left\{ -r \left(\frac{1}{a_0} + ik \right) \right\} r \, dr$$

$$-\frac{1}{ik} \int_0^\infty \exp \left\{ -r \left(\frac{1}{a_0} + ik \right) \right\} r \, dr \right].$$

The integrals in the above can be evaluated by using,

$$\int_0^\infty \exp \left\{-r\alpha\right\} \cdot r^n dr = \frac{n!}{\alpha^{n+1}}.$$
 We obtain,

$$(H_{0}')_{kn} = \frac{2\pi e E_{0} \cos \theta}{\sqrt{(\pi a_{0}^{3} L^{3})}} \times \left[\frac{1}{k^{2} \left(\frac{1}{a_{0}} + ik\right)^{2}} - \frac{2}{ik\left(\frac{1}{a_{0}} - ik\right)^{3}} - \frac{1}{k^{2} \left(\frac{1}{a_{0}} - ik\right)^{2}} - \frac{2}{ik\left(\frac{1}{a_{0}} + ik\right)^{3}} \right]$$

$$= \frac{2\pi e E_0 \cos \theta}{\sqrt{(\pi a_0^3 L^3)}} \times \frac{16k a_0^5}{i(1+a^2 k^2)^3}.$$
 ...(xi)

Substitution of this matrix element, together with the expression (vii) for ρ (k), into (vi) gives the probability per unit time that the electron of the hydrogen atom is ejected into the solid angle $d\Omega$

$$w = \frac{256mk^3e^2E_0^2a_0^7\cos^2\theta}{\pi\hbar^3(1+k^2a_0^2)^6} \cdot d\Omega. \qquad ...(xii)$$

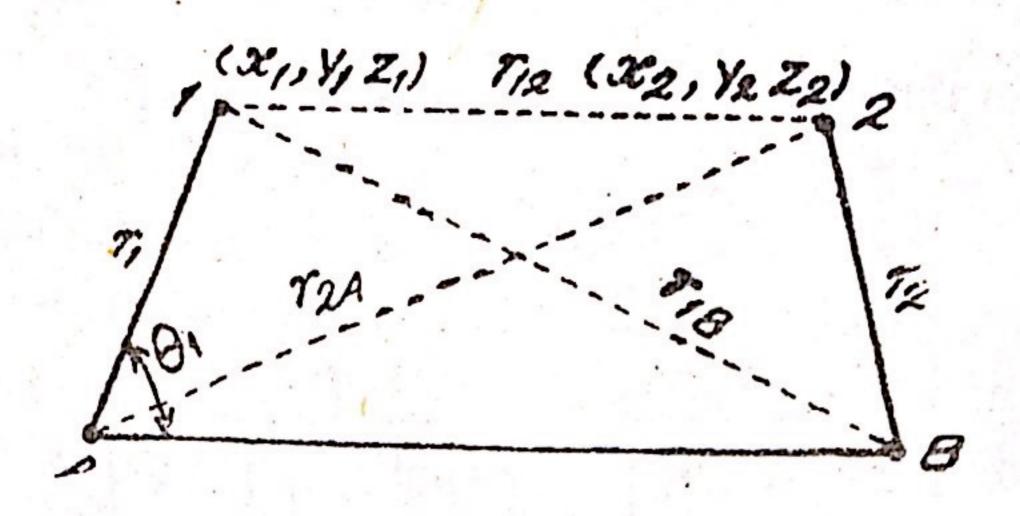
The threshold energy to ionize the atom is the energy required just to remove the electron from the atom, which is equal to the binding energy of the electron in the atom. Since the binding energy of the electron in the state ψ_{200} is lesser than that in the state ψ_{100} , the threshold energy required to ionize the atom from the state ψ_{200} is less.

Problem 9. Consider the interaction between two hydrogen atoms in their ground state (known as Van der Waal's interaction). Obtain an estimate for this energy by applying the second order perturbation theory.

Sol. Let us assume that the nuclei A and B of the hydrogen atoms are fixed in space at a distance R apart and that the z-axis is chosen parallel to the line AB through A and B. I and 2 are the two electron which are at a distance of r_1 and r_2 from A and B; respectively (see Fig. on page 356). r_{12} represents the distance between the two electrons, r_{1B} is the distance of electron 1 from the nucleus B and similarly r_{2A} is the distance of electron 2 from the nucleus A. Hence the Hamiltonian for the system can be written as

$$H = -\frac{\hbar^2}{2m} \left(\nabla_1^2 + \nabla_2^2 \right) - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{R} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}}$$

$$= H_0 + H', \qquad \dots (i)$$



where

$$H_0 = -\frac{\hbar^2}{2m} \left(\nabla_1^2 + \nabla_2^2 \right) - \frac{e^2}{r_1} - \frac{e^2}{r_2} \qquad ...(ii)$$

$$H_0 = -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) - \frac{e^2}{r_1} - \frac{e^2}{r_2} \qquad ...(ii)$$
and $H' = \frac{e^2}{R} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}}$...(iii)
Solution for the next to 1777 to

Solution for the unperturbed Hamiltonian H_0 is the solution,

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \psi_{100}(\mathbf{r}_1) \ \psi_{100}(\mathbf{r}_2), \qquad \dots (iv)$$

for two non-interacting hydrogen atoms in their ground states. We regard the terms H' as a perturbation; which is equivalent to assuming that $R > a_0$,

Since r is much smaller than R, we can write

$$\frac{1}{r_{1B}} = \frac{1}{|\mathbf{r_1} - \mathbf{R}|} = (r_1^2 + R^2 - 2r_1 R \cos \theta_1)^{-1/2}$$

$$= \frac{1}{R} \left(1 - \frac{2z_1}{R} + \frac{r_1^2}{R^2} \right)^{-1/2} (\because z_1 = r_1 \cos \theta_1) \dots (\mathbf{v})$$

Similarly,

$$\frac{1}{r_{2A}} = \frac{1}{R} \left(1 + \frac{2z_{2}}{R} + \frac{r_{2}^{2}}{R^{2}} \right)^{-1/2} \dots (vi)$$

and
$$\frac{1}{r_{12}} = \frac{1}{R} \left[1 + \frac{2(z_2 - z_1)}{R} + \frac{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}{R^2} \right]^{-1/2}$$
.

...(vii)

Using (v), (vi) and (vii), we get

$$H' = \frac{e^2}{R} + \frac{e}{R} \left[1 + \frac{2(z_2 - z_1)}{R} + \frac{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}{R^3} \right]^{-1/2}$$

$$- \frac{e^2}{R} \left[1 + \frac{2z_2}{R} + \frac{r_2^2}{R^2} \right]^{-1/2} - \frac{e^2}{R} \left[1 - \frac{2z_1}{R} + \frac{r_1^2}{R^2} \right]^{-1/2}$$

$$\approx \frac{e^2}{R^3} (x_1 x_2 + y_1 y_2 - 2z_1 z_2). \qquad \dots \text{(viii)}$$

Since H' is an odd function of r_1 and r_2 and ψ_0 (r_1, r_2) is an even function of r_1 and r_2 , the expectation value of H' for ψ_0 (r_1, r_2) vanishes. Hence the first order contribution to the interaction

energy is zero. The second order perturbation gives the contribution,

$$E_2 = \sum_{n}' \frac{|\langle 0 | H' | n \rangle|^2}{E_0 - E_n}(ix)$$

Now
$$\sum_{n=1}^{n} |\langle 0 | H' | n \rangle|^2 = \sum_{n=1}^{n} |\langle 0 | H' | n \rangle|^2 - (\langle 0 | H' | 0 \rangle)^2$$

$$=\langle 0 \mid H'^2 \mid 0 \rangle - (\langle 0 \mid H' \mid 0 \rangle)^2.$$

Since $\langle 0 \mid H' \mid 0 \rangle = 0$, we have

$$\sum_{n} |\{0 \mid H' \mid n\}|^{2} = \langle 0 \mid H'^{2} \mid 0\}. \qquad ...(x)$$

We can obtain an upper limit of E_2 by replacing each E_n in (ix) by E_n^* , the energy of the lowest excited state of the two hydrogen atoms. Then the denominator can be taken outside of the summation and using (x), we can write

$$-E_2 \leqslant \frac{\langle 0 \mid H'^2 \mid 0 \rangle}{E_n^* - E_0}$$
 ...(xi)

From (viii), we have

$$H'^{2} = \frac{e^{4}}{R^{6}} (x_{1}^{2}x_{2}^{2} + y_{1}^{2}y_{2}^{2} + 4z_{1}^{2}z_{2}^{2} + 2x_{1}x_{2}y_{1}y_{2} - \dots) \qquad \dots (xii)$$

The matrix element of the cross-product terms like $x_1x_2y_1y_2$ between the states ψ_0 (\mathbf{r}_1 , \mathbf{r}_2) is zero, since these terms are odd functions of one of the cartesian components of \mathbf{r}_1 or \mathbf{r}_2 . For the first term in (xii) we have,

$$\int x_1^2 x_2^2 \mid \psi_{100} (\mathbf{r}_1) \psi_{100} (\mathbf{r}_2) \mid^2 d^3 r_1 d^3 r_2$$

$$= \frac{1}{3} \int r_1^2 \mid \psi_{100} (\mathbf{r}_1) \mid^2 d^3 r_1 \times \frac{1}{3} \int r_2^2 \mid \psi_{100} (\mathbf{r}_2) \mid^2 d^3 r_2.$$

$$= \frac{1}{9} \left(\int r^2 \mid \psi_{100} (\mathbf{r}) \mid^2 d^3 r \right)^2$$

$$= \frac{1}{9} \left(\frac{4\pi}{\pi a_0^3} \int_0^\infty e^{-2r/a_0} r^4 dr \right)^2$$

$$= \frac{1}{9} \left(\frac{4}{a_0^3} \cdot \frac{4!}{(2/a_0)^5} \right)^2 \left[\because \int_0^\infty e^{-\alpha x} x^n dx = \frac{n!}{x^{n+1}} \right]$$

$$= \frac{1}{9} (3a_0^2)^2 = a_0^4 \qquad \dots (xiii)$$

Similarly, we can find the expectation values of the second and the third terms in (xii). Thus have

$$\langle 0 \mid H'^2 \mid 0 \rangle = \frac{e^4}{R^6} (a_0^4 + a_0^4 + 4a_0^4) = 6 e^4 a_0^4 / R^6 \dots (xiv)$$

The state n^* is the state in which both of the atoms are excited to the state n=2, Therefore $E_0=-2$ ($e^2/2a_0$), $E_n^*=-2$ ($e^2/8a_0$) and, $E_n^*-E_0=3e^2/4a_0$. Hence from (xiv) and (xi) we have

 $E_2 \geqslant -\frac{8e^2a_0^5}{R^6}$ (xv)

Problem 10. A one-dimensional harmonic oscillator is subjected to a constant force F. Classically, its motion is unaffected, except for a displacement of the equilibrium position. Solve the corresponding quantum-mechanical problem by the perturbation method, and compare the result with the exact solution.

Sol. The constant force gives a contribution to the potential energy as

$$-F\int dx = -Fx$$

Hence the Hamiltonian can be written as

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 - Fx = H_0 + H'$$

where Ho is the unperturbed Hamiltonian,

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \qquad ...(i)$$

we treat H' as a perturbation to the Hamiltonian H_0 ,

$$H' = -Fx \qquad ...(ii)$$

Hence the change in the energy levels due to this perturbation, in the first order, is given by

$$E_1 = \langle n \mid H' \mid n \rangle = \int \psi_n^* (x) (-Fx) \psi_n (x) dx$$

$$= -F \int \psi_n^* (x) x \psi_n (x) dx \dots (iii)$$

Here $\psi_n(x)$ is the unperturbed harmonic oscillator wavefunction for the *n*th energy state,

$$\psi_n(x) = \frac{\alpha^{1/2}}{\sqrt{\{2^n \ n \ ! \ \sqrt{(\pi)}\}}} e^{-\alpha^2 x^2/2} H_n(\alpha x) \ ; \alpha^4 = \frac{mk}{\hbar^2} \text{ and } \omega^2 = \frac{k}{m},$$
 ...(iv)

where $H_n(\alpha x)$ is the nth degree Hermite polynomial.

It can be shown that (see prob. 4, chapter-6)

$$\int \psi_n^* (x) \ x \ \psi_m (x) \ dx = \begin{cases} \frac{1}{\alpha} \sqrt{\left(\frac{n+1}{2}\right)} \text{ for } m = n+1\\ \frac{1}{\alpha} \sqrt{\left(\frac{n}{2}\right)} \text{ for } m = n-1\\ \text{otherwise} \end{cases} \dots (v)$$

Thus $E_1=0$, i.e. there is no change in the energy levels in the first order due to a constant force F acting on the oscillator. Therefore, we go to the second order perturbation calculations. The second order change in the unberturbed energy $E_n=(n+\frac{1}{2})$ $\hbar\omega$ is given by

$$E_{2} = \sum_{m}' \frac{(n \mid H' \mid m)|^{2}}{E_{n}^{(0)} - E_{m}^{(0)}} = F^{2} \sum_{m}' \frac{(n \mid x \mid m)|^{2}}{E_{n}^{(0)} - E_{m}^{(0)}} \dots \text{(vi)}$$

Using (v) we have

$$E_{2} = F^{2} \frac{|\langle n \mid x \mid n+1 \rangle|^{2}}{E_{n}^{(0)} - E_{n+1}^{(0)}} + F^{2} \frac{|\langle n \mid x \mid n-1 \rangle|^{2}}{E_{n}^{(0)} - E_{n-1}^{(0)}}$$

$$=E^{2}\frac{\frac{1}{\alpha^{2}}\frac{n+1}{2}}{-\hbar\omega}+F^{2}\frac{\frac{1}{\alpha^{2}}\frac{n}{2}}{\hbar\omega}=-\frac{F^{2}}{2\hbar\omega\alpha^{2}}=\frac{-F^{2}}{2m\omega^{2}}$$
...(vii)

Therefore, we see that the energy of state $\psi_n(x)$ is decreased by a constant value $-F^2/2m\omega^2$ when the oscillator is subjected to a constant force F.

Problem 11. Calculate the first order shift in the zero point energy for a one dimensional anharmonic oscillator described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + ax^4,$$

where the ground state wavefunction for the harmonic oscillator is given by

$$\psi_0(x) = Ne^{-m\omega x^2/2\hbar},$$

N being the normalization constant.

Sol. We can write the Hamiltonian as,

$$H = H_0 + H'$$
; $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ and $H' = ax^4$.

Hence the first order shift in the zero point energy is given by

$$\triangle E_0 = \int \psi_0^*(x) H' \psi_0(x) dx = aN^2 \int_{-\infty}^{+\infty} e^{-(m\omega/\hbar)x^2} x^4 dx.$$

$$=aN^{2}\left(\frac{\hbar}{m\omega}\right)^{5/2}\int_{-\infty}^{+\infty}e^{-t^{2}}t^{2\cdot 2}dt=aN^{2}\left(\frac{\hbar}{m\omega}\right)^{5/2}\cdot\frac{3}{4}\sqrt{(\pi)}, \quad ...(i)$$

where we have used the general formula

$$\int_{-\infty}^{+\infty} x^{2n} e^{-x^2} dx = \frac{1 \cdot 3 \cdot 5 \dots (2n-1)\sqrt{(\pi)}}{2^n}.$$
 (ii)

Now to evaluate the normalization constant N, we have

$$\int_{-\infty}^{+\infty} \psi_0^* (x) \psi_0(x) dx = 1$$
or $N^2 \int_{-\infty}^{+\infty} \exp \left\{ -\frac{m\omega}{\hbar} x^2 \right\} dx = 1$
or $N^2 \sqrt{\left(\frac{\hbar}{m\omega}\right)} \int_{-\infty}^{+\infty} e^{-t^2} dt = 1$
or $N^2 \sqrt{\left(\frac{\hbar}{m\omega}\right)} \cdot \sqrt{(\pi)} = 1 \quad \left\{ \begin{array}{c} : \int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{(\pi)} \right\} \\ \Rightarrow N^2 = \sqrt{\left(\frac{m\omega}{\hbar \pi}\right)} & \dots \text{(iii)} \end{array}$

Using it into (i) we have

$$\Delta E_0 = a \sqrt{\left(\frac{m\omega}{\hbar\pi}\right)} \cdot \left(\frac{\hbar}{m\omega}\right)^{5/2} \cdot \frac{3}{4} \sqrt{(\pi)} = \frac{3a}{4} \left(\frac{\hbar}{m\omega}\right)^2 \dots (iv)$$

Hence the zero point energy is increased by the amount

$$\frac{3a}{4} \left(\frac{\hbar}{m\omega}\right)^2$$

Problem 12. The interaction V(x) is added to the Hamiltonian $(p^2+m^2\omega^2x^2)/2m$. Calculate by the perturbation theory the first and second order energy level shifts for the following two cases:

(a)
$$V(x) = \frac{1}{2} m\omega^2 x^2$$

(b)
$$V(x) = bx^3$$

Sol. The Hamiltonian $H_0=(p^2+m^2\omega^2x^2)/2m$ represents a simple harmonic oscillator, the Schroedinger equation for which can be solved exactly. The eigenvalues and eigenfunctions of H_0 are:

$$E_{n} = (N + \frac{1}{2}) \hbar \omega : \qquad n = 0, 1, 2, ...$$

$$\psi_{n}(x) = \frac{\alpha^{1/2}}{\sqrt{\{2^{n} n! \sqrt{(\pi)}\}}} e^{-\alpha^{2} x^{2} / 2} H_{n}(\alpha x); \quad \alpha^{6} = \frac{m^{2} \omega^{2}}{\hbar^{2}} ...(ii)$$
The Halis the with Harmitan 1...(ii)

where H_n is the nth Hermite polynomial.

Now treating V(x) as a perturbation to H_0 we can calculate the energy shift in the level E_n due to this interaction. For the perturbation calculation we need to find the matrix elements for x^2 and x^3 . For it we have the matrix element of x, between two harmonic oscillator states n and m as (see prob. 4, Chapter-6)

$$\langle n \mid x \mid m \rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} [\sqrt{(n+1)} \, \delta_{n+1}, \, m + \sqrt{(n)} \, \delta_{n-1}, \, m] \dots \text{(iii)}$$

To find the matrix elements for x^2 we have

$$\langle n \mid x^2 \mid m \rangle = \sum_{i} \langle n \mid x \mid t \rangle \langle t \mid x \mid m \rangle$$

$$= \frac{\hbar}{2m\omega} \sum_{t} \{ \sqrt{(n+1)} \, \delta_{n+1}, \, t + \sqrt{(n)} \, \delta_{n-1}, \, t \} \{ \sqrt{(t+1)} \, \delta_{t-1}, \, m \}$$

$$= \frac{\hbar}{2m\omega} \left[\sqrt{\{(n+1)(n+2)\}} \, \delta_{n+2}, \, m + \sqrt{\{n \, (n-1)\}} \, \delta_{n-2}, \, m \right]$$

$$+ (2n+1) \, \delta_{nm} \right] \dots (iv)$$
Similarly,
$$\langle n \mid x^3 \mid m \rangle = \sum_{t} \langle n \mid x^2 \mid t \rangle \langle t \mid x \mid m \rangle$$

$$= \left(\frac{\hbar}{2m\omega} \right)^{3/2} \sum_{t} \left[\sqrt{\{(n+1) \, (n+2)\}} \, \delta_{n+2}, \, t + \sqrt{\{n(n-1)\}} \, \delta_{n-2}, \, t \right]$$

$$+ (2n+1) \, \delta_{nt} \right] \left[\sqrt{\{t+1\}} \, \delta_{t+1}, \, m + \sqrt{\{t\}} \, \delta_{t-1}, \, m \right]$$

$$= \left(\frac{\hbar}{2m\omega} \right)^{3/2} \left[\sqrt{\{(n+1)(n+2)(n+3)\}} \, \delta_{n+3}, \, m + (3n+3)\sqrt{\{n+1\}} \right]$$

$$\times \delta_{n+1}, \, m+3n\sqrt{(n)} \, \delta_{n-1}, \, m+\sqrt{\{n(n-1) \, (n-2)\}} \, \delta_{n-3}, \, m \right] \dots (v)$$
For the case (a), first order energy shift to the energy E is

For the case (a), first order energy shift to the energy E_n is given by:

$$E_{1} = \langle n \mid H_{1}' \mid n \rangle = \frac{1}{2}m\omega^{2} \langle n \mid x^{2} \mid n \rangle$$

$$= \frac{1}{2}m\omega^{2} \cdot \frac{\hbar}{2m\omega} (2n+1) \quad \text{[Using (iv)]}$$

$$= \frac{\hbar\omega}{4} (2n+1)$$

$$= (n+\frac{1}{2}) \frac{\hbar\omega}{2}$$
For the second and and if ω ... (vi)

For the second order shift we have,

$$E_{2} = \sum_{m} \frac{\langle n \mid x^{2} \mid m \rangle \langle m \mid x^{2} \mid n \rangle}{E_{n} - E_{m}}$$

$$= \left(\frac{\hbar}{2m\omega}\right)^{2} \left[\frac{(n+1)(n+2)}{-2\hbar\omega} + \frac{n(n-1)}{2\hbar\omega}\right]$$

$$= -\left(\frac{\hbar}{2m\omega}\right)^{2} \cdot \frac{1}{2\hbar\omega} \left[(n+1)(n+2) - n(n-1)\right]$$

$$= -\frac{\hbar}{8m^{2}\omega^{3}} \cdot (4n+2)$$
(vii)

For the case (b), first order energy shift is zero because we see from (v) that $\langle n \mid x^3 \mid n \rangle = 0$. For the second order shift we have, $E_2 = \sum \frac{\langle n \mid x^3 \mid m \rangle \langle m \mid x^3 \mid n \rangle}{E_n - E_m} = \left(\frac{\hbar}{2m\omega}\right)^3 \left[\frac{(n+1)(n+2)(n+3)}{-3\hbar\omega}\right]$

$$E_{n}-E_{m} = \frac{1}{2m\omega} \left[\frac{(n+1)(n+2)(n+2)(n+2)(n+2)(n+2)}{-3\hbar\omega} + \frac{9(n+1)^{3}}{-\hbar\omega} + \frac{9n^{3}}{\hbar\omega} + \frac{n(n-1)(n-2)}{3\hbar\omega} \right]$$

$$= \frac{15}{4} \left(\frac{\hbar}{m\omega}\right)^3 \frac{1}{\hbar\omega} \left(n^2 + n + \frac{11}{30}\right) \qquad ...(viii)$$

Problem 13. If Φ is a single-valued continuous function, and $\Phi^*\Phi d^3r=1$, then show that

$$\int \Phi^* H \Phi \ d^3r \geqslant E_0,$$

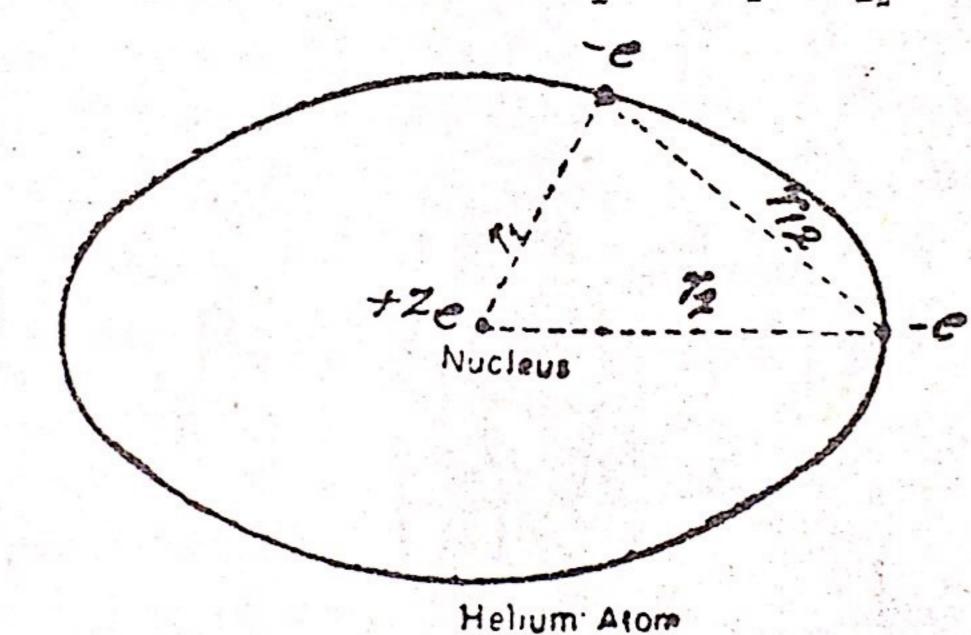
where, operator H has only a discrete spectrum, and E_0 is the lowest energy value of H.

Assuming
$$\Phi = \frac{Z^3}{\pi a_0^3} \exp \left[-Z (r_1 + r_2)/a_0 \right],$$

obtain an expression for the energy of the ground state of a helium like atom $(r_1 \text{ and } r_2 \text{ being the distances of the electrons from the})$ nucleus).

The helium atom consists of a nucleus of charge + Ze (where Z=2) and two electrons each of charge -e as shown in the figure below. The Hamiltonian for the system can be written as

$$H = -\frac{\hbar^2}{2m} \left(\nabla_1^2 + \nabla_2^2 \right) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}} \qquad .. (i)$$



In order to find the ground state energy we use the Variational Method. For it we consider the quantity z as a variational parameter z' instead of a constant equal to the atomic number. According to the the variational method we compute the expectation value $\langle H \rangle$ of the Hamiltonian w.r.t. the trial wave function ϕ , and then minimize $\langle H \rangle$ w.r.t. the variational parameter z'. The minimum value of $\langle H \rangle$ gives an estimate of the ground state energy.

Now we write ϕ as

$$\phi = \sqrt{\left(\frac{z'^3}{\pi a_0^3}\right)} \exp \left[-z'r_1/a_0\right] \times \sqrt{\left(\frac{z'^3}{\pi a_0^3}\right)} \exp \left[-z'r_2/a_0\right] = \phi_1\phi_2, \quad \dots \text{(ii)}$$

Functions ϕ_1 and ϕ_2 in the above are hydrogen like wave-functions for the nuclear charge z' e. Hence we have

$$\left(-\frac{\hbar^{2}}{2m}\nabla_{1}^{2} - \frac{z'e^{2}}{r_{1}}\right)\phi_{1} = E_{H}\phi_{1} \qquad ...(iii)$$

$$\left(-\frac{\hbar^{2}}{2m}\nabla_{2}^{2} - \frac{z'e^{2}}{r_{2}}\right)\phi_{2} = E_{H}\phi_{2} \qquad ...(iv)$$

and

where $E_H = -z'^2 e^2/2a_0$ is the ground state energy for the hydrogen atom. Using (iii) and (iv) we get

$$\langle H \rangle = \int \phi^* H \phi d^3 r = \int \phi_1^* \phi_2^* \left[-\frac{\hbar^2}{2m} \left(\nabla_1^2 + \nabla_2^2 \right) \right. \\ \left. - \frac{ze^2}{r_1} - \frac{ze^2}{r_2} + \frac{e^2}{r_{12}} \right] \phi_1 \phi_2 \ d^3 r_1 \ d^3 r_2$$

$$= -\frac{2z'^2 e^2}{2a_0} + (z' - z) \ e^2 \int \phi_1^* \phi_2^* \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \phi_1 \phi_2 \ d^3 r_1 \ d^3 r_2$$

$$+ e^2 \int \phi_1^* \phi_2^* \frac{1}{r_{12}} \phi_1 \phi_2 \ d^3 r_1 \ d^3 r_2$$
 ...(v)
$$\text{Now } \int \phi_1^* \phi_2^* \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \phi_1 \phi_2 \ d^3 r_1 \ d^3 r_2 = 2 \int \phi_1^* \frac{1}{r_1} \phi_1 \ d^3 r_1$$

$$= 2. \frac{z'^3}{\pi a_0^3} \int \frac{1}{r_1} \exp \left[-2z' \ r_1 / a_0 \right] \ r_1^2 \ dr_1 \sin \theta_1 \ d\theta_1 \ d\phi_1$$

$$= 2. 4\pi . \frac{z'^3}{\pi a_0^3} \int_0^\infty \exp \left[-2z' r_1 / a_0 \right] r_1 \ dr_1$$

$$= 2. 4\pi . \frac{z'^3}{\pi a_0^3} . \frac{1}{(2r'/a_0)^2}$$

$$\left[\therefore \int_0^\infty \exp \left[-\alpha x \right] x^n dx = \frac{n!}{\alpha^{n+1}} \right]$$

$$= \frac{2r'}{a_0}$$
 ...(vi)

Next we consider the interaction integral,

$$\left(\frac{z'^3}{\pi a_0^3}\right)^2 \iint \frac{e^2}{r_{12}} \exp \left[-2z' \left(r_1+r_2\right)/a_0\right] d^3r_1 d^3r_2$$

Consider first the integration over r_2 , keeping r_1 fixed. The relevant part of the integral is

$$\int \frac{1}{r_{12}} \exp \left[-2z' r_2 / a_0 \right] d^3 r_2 = \int_0^\infty r_2^2 dr_2 \int \sin \theta_2 d\theta_2 d\phi_2$$

$$\exp \left[-2z' r_2 / a_0 \right] \cdot \frac{1}{r_{12}} \dots \text{(vii)}$$

To evaluate (vii), we use the expansions

$$\frac{1}{r_{12}} = \frac{1}{r_1} \sum_{l=0}^{\infty} \left(\frac{r_2}{r_1}\right)^{l} P_l \left(\cos \theta_{12}\right), r_1 > r_2
= \frac{1}{r_2} \sum_{l=0}^{\infty} \left(\frac{r_1}{r_2}\right)^{l} P_l \left(\cos \theta_{12}\right), r_1 < r_2
\dots \text{ (viii)}$$

and choose the polar axis to be along the direction of r_1 so that equal to the polar angle θ_2 is the angle θ_{12} between r_1 and r_2 . Then (vii) becomes

$$\int_{0}^{r_{1}} r_{2}^{2} dr_{2} \int \sin \theta_{2} d\theta_{2} d\phi_{2}$$

$$\exp \left[-2z'r_{2}/a_{0}\right] \left[\frac{1}{r_{1}} \sum_{l=0}^{\infty} \left(\frac{r_{2}}{r_{1}}\right)^{l} P_{l} \left(\cos \theta_{2}\right)\right]$$

$$+ \int_{r_{1}}^{\infty} r_{2}^{2} dr_{2} \int \sin \theta_{2} d\theta_{2} d\phi_{2}$$

$$\exp \left[-2z'r_{2}/a_{0}\right] \left[\frac{1}{r_{2}} \sum_{l=0}^{\infty} \left(\frac{r_{1}}{r_{2}}\right)^{l} P_{l} \left(\cos \theta_{2}\right)\right] \qquad \dots (ix)$$

Since, $\int P_l(\cos \theta_2) \sin \theta_2 d\theta_2 d\phi_2 = 4\pi\delta_{l0}$, only the term with l=0 survives in each integral. Thus (ix) reduces to

$$\int_{0}^{r_{1}} dr_{2} r_{2}^{2} \exp \left[-2z' r_{2}/a_{0}\right] \frac{1}{r_{1}} 4\pi$$

$$+ \int_{r_{1}}^{\infty} r_{2} dr_{2} \exp \left[-2z' r_{2}/a_{0}\right] 4\pi$$

$$= -\frac{a_{0}^{2}}{4z'^{2}} \left[1 + \frac{a_{0}}{2z' r_{1}}\right] \exp \left[-2z' r_{1}/a_{0}\right] + \frac{a_{0}^{3}}{4z'^{3} r_{1}}$$
Using this value of (vii) and(x)

Using this value of (vii) and carrying out the r_1 integration, we finally get

$$\left(\frac{z'^3}{\pi a_0^3}\right)^2 \iint \frac{e^2}{r_{12}} \exp\left[-2z' \left(r_1 + r_2\right)/a_0\right] d^3r_1 d^3r_2$$

$$= \frac{5e^2 z'}{8a_0}$$

$$\therefore \langle H \rangle = -\frac{2z'^2e^2}{2a_0} + \frac{2z' \left(z' - z\right) e^2}{a_0} + \frac{5z' e^2}{8a_0} \qquad \dots (xi)$$
For $\langle H \rangle$

...(xii)

For $\langle H \rangle$ to be minimum, z' should be such that

$$\frac{\partial \langle H \rangle}{\partial z'} = \frac{-4z'e^2}{2a_0} + \frac{4z'e^3}{a_0} - \frac{2ze^2}{a_0} + \frac{5e^2}{8a_0} = 0$$

$$-2z' + 4z' - 2z + \frac{5}{8} = 0$$

$$z'=z-\frac{5}{16}=2-\frac{5}{16}=\frac{27}{16}$$
 ...(xiii)

Which leads to

$$\langle H \rangle_{min} = -2.85 \ e^2/a_0$$

The hydrogen-like wavefunctions give the best energy value z'=27/16 rather than 2.

Problem 14. Obtain an approximate value for the lowest energy of the hydrogen atom using variational method with the wavefunction,

$$\psi = \sqrt{\left(\frac{a^3}{\pi}\right)} e^{-ar}$$

as a trial function.

Sol. For the ground state of hydrogen atom, we have the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{r} \qquad \dots (i)$$

The value of ∇²ψ is given by

$$\nabla^{2}\psi = \sqrt{\left(\frac{a^{3}}{\pi}\right)\left[\frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial}{\partial r}\right)\right]}e^{-ar}$$

$$= \frac{1}{r^{2}}\left[2r\frac{\partial}{\partial r}\left(e^{-ar}\right) + r^{2}\frac{\partial^{2}}{\partial r^{2}}\left(e^{-ar}\right)\right]\sqrt{\left(\frac{a^{3}}{\pi}\right)}$$

$$= \frac{1}{r^{2}}\left[2r\left(-a\right)e^{-ar} + r^{2}a^{2}e^{-ar}\right]\sqrt{\left(\frac{a^{3}}{\pi}\right)}$$

$$= e^{-ar}\left(a^{2} - \frac{2a}{r}\right)\sqrt{\left(\frac{a^{3}}{\pi}\right)}$$

$$\langle H \rangle = \int \psi^{*}\left(-\frac{\hbar^{2}}{2m}\nabla^{2} - \frac{e^{2}}{r}\right)\psi d^{3}r$$

$$= 4\pi\frac{a^{3}}{\pi}\left[\int_{0}^{\infty}\exp\left(-2ar\right)\left\{-\frac{\hbar^{2}}{2m}\left(a^{2} - \frac{2a}{r}\right)\right\}\right]$$

$$\times r^{2}dr - 4\pi e^{2}\frac{a^{3}}{\pi}\int_{0}^{\infty}\exp\left(-2ar\right)\left[-2ar\right]\frac{1}{r}r^{2}dr\right]$$

$$= -\frac{2\hbar^{2}a^{5}}{m}\int_{0}^{\infty}\exp\left(-2ar\right)rdr - 4e^{2}a^{3}\int_{0}^{\infty}\exp\left(-2ar\right)rdr$$

$$= -\frac{2\hbar^{2}a^{5}}{m}\cdot\frac{2!}{(2a)^{3}} + \frac{8a^{4}\hbar^{2}}{2m}\cdot\frac{1}{(2a)^{2}} - 4e^{2}a^{3}\cdot\frac{1}{(2a)^{2}}$$

$$= \frac{n^2 a^2}{2m} - e^2 a \qquad(ii)$$

Now we shall choose a in such a way that $\langle H \rangle$ is minimized.

For it we have

$$\frac{\partial \langle H \rangle}{\partial a} = \frac{\hbar^2 a}{m} - e^2 = 0 \Rightarrow a = \frac{me^2}{\hbar^2} \qquad ...(iii)$$

Substituting this value of a into (ii) we get the ground state energy of hydrogen as:

$$\langle H \rangle_{min} = \frac{\hbar^2 \cdot m^2 e^4}{2m \cdot \hbar^4} - \frac{me^4}{\hbar^2} = -\frac{me^4}{2\hbar^2} \qquad ...(iv)$$

This is exactly same the as we got by solving the Schroedinger equation for the hydrogen atom in chapter 6.

It is left as an exercise for the readers to find the lowet energy of hydrogen with the trial function,

$$\psi = \left(\frac{2a}{\pi}\right)^{3/4} \exp.(-ar^2).$$

To evalute the integrals use the result,

$$\int_{-\infty}^{+\infty} x^{2n} e^{-x^2} dx = \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)\sqrt{\pi}}{2^n} \dots (v)$$

Problem 15. Apply the variational method to estimate the ground state energy of the deutron. The ground state wave function is spherically symmetrical, and the neutron and the proton are assumed interact through the Yukawa potential

$$V(r) = -V_0 e^{-r/r_0} / \left(\frac{r}{r_0}\right), \qquad ... (i)$$

where V_0 and r_0 are constants.

Sol. In the centre-of-mass coordinates, the Himiltonian for the ground state of the neutron-proton system is given by

$$H = \frac{p^2}{2m} + V(r), \qquad \dots (ii)$$

where m is the reduced mass of the $n \cdot p$ system and V(r) is given by Gby (i).

For the variational calculation of the ground state energy of the deutron, we use the simple trial function

 $\psi = e^{-\alpha r/r_0}$: In which we treat α as a variational parameter. For convenience, We introduce the variable $x = \frac{r}{r}$, and obtain

$$\langle H \rangle = \frac{\int_{0}^{\psi^{*}} \frac{p^{2}}{2m} \psi d^{3}r + \int_{0}^{\psi^{*}} V(r) \psi d^{3}r}{\int_{0}^{\psi^{*}} \psi d^{3}r} \dots (iv)$$
Now,
$$\int_{0}^{\psi^{*}} \psi d^{3}r = 4\pi \int_{0}^{\infty} e^{-2\alpha r/r_{0}} r^{2} dr$$

$$= 4\pi r_{0}^{3} \int_{0}^{\infty} e^{-2\alpha x} x^{2} dx = \frac{\pi r^{3}}{\alpha^{3}}; \dots (v)$$

$$\int_{0}^{\psi^{*}} \frac{p^{2}}{2m} \psi d^{3}r = \frac{\hbar^{2}}{2m} \int_{0}^{\psi^{*}} \psi \frac{d^{2}\psi}{dr^{2}} d^{3}r = \frac{\hbar^{2}}{2m} \frac{\alpha^{2}}{2m} 4\pi \int_{0}^{\infty} e^{-2\alpha r/r_{0}} r^{2} dr$$

$$= \frac{\hbar^{3}}{2m} \cdot \frac{\alpha^{2}}{r_{0}^{2}} \cdot 4\pi \cdot r_{0}^{2} \int_{0}^{\infty} e^{-2\alpha x} x^{2} dx = \frac{\hbar^{2}r_{0}}{2m} \frac{\pi}{\alpha} \dots (vi)$$
and
$$\int_{0}^{\psi^{*}} V(r) \psi d^{3}r = -V_{0} \cdot 4\pi \int_{0}^{\infty} e^{-r} \frac{e^{-2\alpha r/r_{0}}}{r/r_{0}} e^{-2\alpha r} r^{2} dr$$

 $\int_{0}^{\pi} V(r) \psi \, d^{3}r = -V_{0} \cdot 4\pi \int_{0}^{\pi} \frac{e^{-2r}}{r/r_{0}} e^{-2r/r_{0}} r^{2} \, dr$ $= -V_{0} \cdot 4\pi r_{0}^{3} \int_{0}^{\infty} \frac{e^{-x}}{x} \cdot e^{-2\alpha x} \cdot x^{2} \, dx$ $= -V_{0} \cdot 4\pi r_{0}^{3} \frac{1}{(2\alpha + 1)^{2}} \qquad \dots \text{(vii)}$

For evaluating (v), (vi) and (vii) we have used the general result

$$\int_0^\infty e^{-\alpha x} x^n dx = \frac{n!}{\alpha^{n+1}}$$

Using these results into (iv) we find that:

$$\langle H \rangle = \left[\frac{\hbar^2 r_0 \pi}{2m\alpha} - \frac{V_0 4\pi r_0^3}{(2\alpha + 1)^2} \right] / \frac{\pi r_0^3}{\alpha^3} = \frac{\hbar^2}{2m} \cdot \frac{\alpha^2}{r_0^2} - \frac{4V_0 \alpha^3}{(\alpha + 1)^2} \dots \text{(viii)}$$

The best approximation is obtained by minimizing the expression (viii) with respect to α . For it we have,

$$\frac{\partial \langle H \rangle}{\partial \alpha} = \frac{\hbar^2}{2m} \frac{2\alpha}{r_0^2} - 4V_0 \frac{[(2\alpha+1)^2 \cdot 3\alpha^2 - \alpha^3 \cdot 4(2\alpha+1)]}{(2\alpha+1)^4} = 0$$

$$\frac{\alpha}{(2\alpha+1)^3} = \frac{\hbar^2}{4m r_0^2 V_0} \dots (ix)$$

Hence, for the minimum value of $\langle H \rangle$, α should satisfy equation (ix) and for this value of α ,

$$\langle H \rangle_{min} = -\frac{\hbar^2 \alpha^2 (2\alpha - 1)}{2mr_0^2 (2\alpha + 3)} \dots (x)$$

If the quantities V_0 and r_0 are given, the corresponding value of $\langle H \rangle_{min}$ can be found by solving equation (ix) for α and substituting it into eqn (x).

It is left as an exercise for the readers to evaluate the value $\langle H \rangle_{min}$ with the trial function

where
$$\beta$$
 is an additional variational parameter ...(xi)

where β is an additional variational parameter.

Problem 16. If a trial wavefunction $\psi = \frac{1}{\sqrt{(a)}} \cos \frac{\pi x}{2a}, -a \leq x$ is used in a variational method of approximation for the energy of a one-dimensional harmonic oscillator, $H=(p^2+m^2\omega^2x^2)/2m$; show that the best value of a^2 is $\left(\frac{\pi \hbar}{2m\omega}\right) \left(\frac{1}{3} - \frac{2}{\pi^2}\right)^{-1/2}$, and the corresponding energy is $\frac{1}{2}\hbar\omega \left(\frac{\pi^2-6}{3}\right)^{1/2}$

Hint. In this problem we encounter two integrals, first one is

$$\int_{-a}^{+a} \cos^2 \frac{\pi x}{2a} = \frac{1}{2} \int_{-a}^{+a} \left(1 + \cos \frac{\pi x}{a} \right) dx = a;$$

and the second, is

 $\int_{-\pi}^{\pi} x^2 \cos^2 \frac{\pi x}{2a} dx$, which can be easily evaluated by parts. The

result of this integral comes out to be $\left(a^3 - \frac{4a^3}{3} - \frac{4a^3}{\pi^2}\right)$.

Problem 17. A particle of mass m is bound by the potential $V(r) = -V_0 e^{-r/a}$ where $\hbar^2/2mV_0a^2 = \frac{8}{4}$. Use the variational method with the trial function $e^{-\alpha r}$ to get a good limit on the lowest energy

The Hamiltonian for the particle is,

$$H = \frac{p^2}{2m} + V(r) = \frac{\hbar^2}{2m} \frac{d^2}{dr^2} - V_0 e^{-r/a} \qquad ...(i)$$

$$\therefore \langle H \rangle = \frac{(\hbar^2 \alpha^2 / 2m) \int_0^\infty 2^{-2\alpha r} d^3 r - V_0 \int_0^\infty e^{-r/a} e^{-2\alpha r} d^3 r}{\int_0^\infty e^{-2\alpha r} d^3 r} \dots (ii)$$

From the standard result, $\int_0^\infty e^{-\alpha x} x^n dx = n!/\alpha^{n+1}$, we have,

$$\int_{0}^{\infty} e^{-2\alpha r} d^{3}r = 4\pi \int_{0}^{\infty} e^{-2\alpha r} r^{2} dr = 4\pi \cdot \frac{2!}{(2\alpha)^{3}} = \frac{\pi}{\alpha^{3}} \qquad \dots \text{(iii)}$$

and $\int_{0}^{\infty} e^{-r/a} \cdot e^{-2\alpha r} d^{3}r = 4\pi \int_{0}^{\infty} \exp\left[-r\left(\frac{1}{a} + 2\alpha\right)\right] r^{2} dr$

$$= 4\pi \frac{2}{\left(\frac{1}{a} + 2\alpha\right)^3} \dots (iv)$$

$$\therefore \langle H \rangle = \left[\frac{\hbar^2 \alpha^2}{2m} \cdot \frac{\pi}{\alpha^3} - \frac{8\pi V_0}{\left(\frac{1}{a} + 2\alpha\right)^3}\right] \frac{\pi}{\alpha^3}$$

$$= \frac{\hbar^2 \alpha^2}{2m} - \frac{8\pi V_0}{\pi} \frac{\alpha^3}{\left(\frac{1}{a} + 2\alpha\right)^3} \dots (v)$$

To get the lowest value of $\langle H \rangle$, α should satisfy the condition,

To get the lowest value of
$$\langle H \rangle$$
, $3\alpha^2 - \alpha^3 \cdot 6\left(\frac{1}{a} + 2\alpha\right)^2$.

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 = \frac{\hbar^2}{2m} \cdot 2\alpha - 8V_0 \frac{\left(\frac{1}{a} + 2\alpha\right)^3 \cdot 3\alpha^2 - \alpha^3 \cdot 6\left(\frac{1}{a} + 2\alpha\right)^2}{\left(\frac{1}{a} + 2\alpha\right)^6}$$
or
$$\frac{\hbar^2}{m} - \frac{24V_0}{a} \cdot \frac{\alpha}{\left(\frac{1}{a} + 2\alpha\right)^4} = 0$$

or
$$\frac{\hbar^2}{2mV_0 a^2} = \frac{24}{a^3} \cdot \frac{\alpha}{\left(\frac{1}{a} + 2\alpha\right)^4}$$

or
$$\frac{3}{4} = \frac{24}{a^3} \cdot \frac{\alpha}{\left(\frac{1}{a} + 2\alpha\right)^4}$$

or
$$\frac{\alpha}{\left(\frac{1}{a} + 2\alpha\right)^4} = \frac{a^8}{32} \qquad \dots \text{(vi)}$$

This equation is satisfied for $\alpha = \frac{1}{2a}$. Putting this value of α into (v) we obtain:

$$\langle H \rangle_{min.} = \frac{\hbar^2}{8ma^2} - \frac{1}{8} V_0 = \frac{\hbar^2}{8ma^2} - \frac{1}{8} \times \frac{4}{3} \cdot \frac{\hbar^2}{2ma^2}$$

$$= \frac{\hbar^2}{24ma^2}. \qquad ...(vii)$$

Problem 18. If the first (n-1) eigenfunctions of a particular Hamiltonian are known, write a formal expression for a variational-method trial function that could be used to get an upper limit on the nth energy level.

[Hint. Such a function is any function orthogonal to the given functions, which can be constructed by the Schmidt orthogonalization process].

Problem 19. Estimate the ground state energy of the anharmonic oscillator $(V=\frac{1}{2}m\omega^2x^2+\lambda x^4)$ by the variational method taking the trial wavefunction to be a linear combination of the n=0 and n=2 eigenfunctions of a harmonic oscillator of angular frequency ω .

Sol. The normalized oscillator functions for n=0 and n=2

are

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \exp\left\{-\frac{m\omega}{2\hbar} x^2\right\}, \text{ and}$$

$$\psi_2 = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \frac{1}{\sqrt{(8)}} \left(\frac{4m\omega}{\hbar} x^2 - 2\right) \exp\left\{-\frac{m\omega}{2\hbar} x^2\right\} \dots (i)$$

The Hamiltonian H for the anharmonic oscillator can be

$$H = \left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2\right) + \lambda x^4 = H_0 + \lambda x^4, \qquad \dots (ii)$$

written as

where H_0 is the Hamiltonian for the simple harmonic oscillator such that $H_0 \psi_0 = \frac{1}{2} \hbar \omega \psi$, and $H_0 \psi_2 = \frac{5}{2} \hbar \omega \psi_2$...(iii)

Now taking the trial wavefunction,

$$\psi = C_0 \psi_0 + C_2 \psi_2, \qquad \dots (iv)$$

we know from equation (106) of the variation method that the ground state energy of the anharmonic oscillator will be the smaller root of the eqn.

$$\begin{vmatrix} H_{00} - \chi \triangle_{00} & H_{02} - \chi \triangle_{02} \\ H_{20} - \chi \triangle_{20} & H_{22} - \chi \triangle_{22} \end{vmatrix} = 0, \qquad \dots(v)$$

where
$$\triangle_{ij} = \int \psi_i^* \psi_j d^3r$$
, and $H_{ij} = \int \psi_i^* H \psi_j d^3r$...(vi)

Since the harmonic oscillator functions are orthonormal, we have

$$\triangle_{00} = \triangle_{22} = 1$$
 and $\triangle_{02} = \triangle_{20} = 0$...(vii)

Also,

$$H_{0,1} = \frac{1}{2} \hbar\omega + \lambda \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{+\infty} \exp\left\{-\frac{m\omega}{\hbar} x^2\right\} x^4 dx$$

$$= \frac{1}{2} \hbar\omega + \frac{3\lambda}{4} \left(\frac{\hbar}{m\omega}\right)^2, \qquad ...(viii)$$

$$H_{22} = \frac{5}{2} \hbar\omega + \frac{39\lambda}{4} \left(\frac{\hbar}{m\omega}\right)^2, \text{ and} \qquad ...(ix)$$

$$H_{02} = H_{20} = \frac{3\lambda}{8\sqrt{(8)}} \left(\frac{\hbar}{m\omega}\right)^2$$
 ...(x)

Using (vii) and evaluating the determinant (v), we get $X^2-(H_{00}+H_{22})$ $X+H_{00}H_{22}-H_{02}H_{20}=0$(xi)

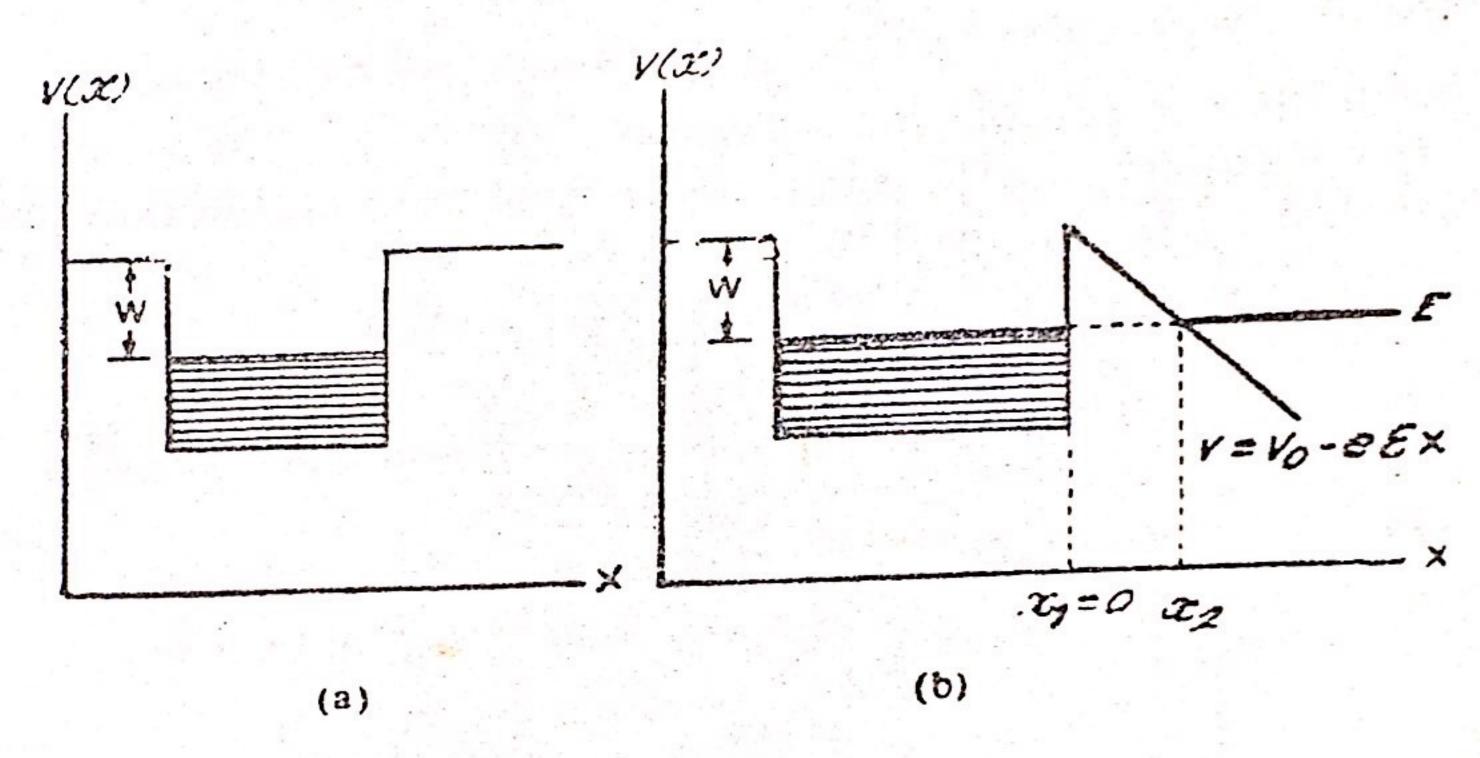
Smaller root of it is,

$$\chi = \frac{1}{2} (H_{00} + H_{22}) - \frac{1}{2} [(H_{00} - H_{22})^2 + 4H_{02}H_{20}]. \qquad ... \text{(xii)}$$

This gives the ground state energy of the anharmonic oscillator, where H_{00} , H_{22} and $H_{02} = H_{20}$ are given by the expressions (viii), (ix) and (x); respectively.

Problem 20. Use WKB method to find out an expression for the probability of emission of electrons from a metal when an external electric field & is applied to the metal.

Sol. In the absence of the electric field &, the electrons are bound by a potential, as shown in fig. (a). The work function W is



the energy required to remove an electron from the highest occupied state

When the external electric field & is applied to the metal, the potential at the surface takes the form indicated in fig. (b). Now the potential barrier has a finite width through which the electrons are able to escape. From equation (158) of this chapter, the probability of transmission through the barrier is given by

$$T^2 = \exp\left(-\frac{2}{\hbar} \int_{x_1}^{x_2} \sqrt{2m (V(x) - E)} dx\right)$$
 ...(i)

Here we set $x_1 = 0$, and then x_2 is given by

$$V_0 - e \mathcal{E} x_2 = V_0 - W$$

$$x_2 = \frac{W}{e \mathcal{E}} \qquad \dots \text{(ii)}$$

Also,
$$(V-E)=V_0-e\mathcal{E}x-E=W-e\mathcal{E}x$$
. ...(iii)
Using (ii) and (iii) into (i), we get

$$T^2 = \exp\left(-\frac{2}{\hbar}\int_0^{W/e\xi} \sqrt{[2m(W-e\xi x)]} dx\right).$$
 ...(iv)

To evaluate this integral, we set $t^2=2m$ (W-eEx). Then

$$T^2 = \exp\left(\frac{2}{me\hbar\epsilon} \int_{\sqrt{(2mW)}}^{0} t^2 dt\right) = \exp\left(-\frac{4}{3} \frac{\sqrt{(2m)}W^{3/2}}{\hbar}\right)...(v)$$

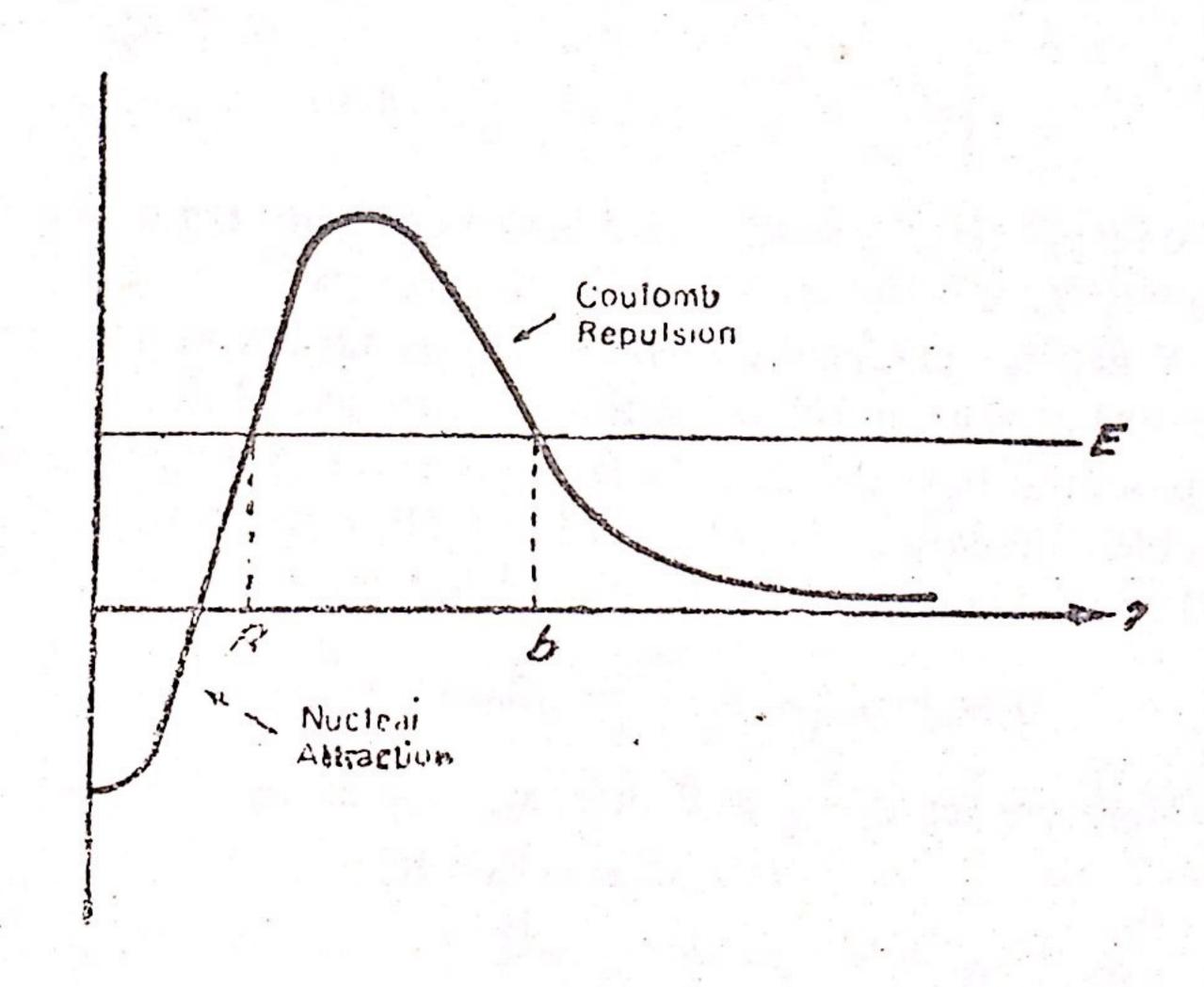
Problem 21. Use WKB method to derive an expression for the half life of a nucleus for a-decay using a simplified radial potential model. The a-particle experiences a strong attractive potential well inside the nucleus and a coulombic barrier outside the well region.

Sol. Let the potential for the α particle (charge ze) which has been emitted from a nucleus of atomic number (Z+z) be V(r). At large distances from the nucleus there is a Coulomb potential $V(r) = \frac{Zze^2}{r}$, where e is the electronic charge and r is the distance between the nucleus and the α -particle.

From equation (158), the probability of transmission through a potential barrier is given by

$$T^2 = \exp\left\{-\frac{2}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V-E)}\right\} dx$$

In our case, the turning points are R and b and $V = \frac{Zze^2}{r}$, $E = V_b = \frac{Zze^2}{h}$; therefor



$$T^{2} = \exp \left\{ -\frac{2}{\hbar} \int_{R}^{b} \sqrt{\left[2m \left(\frac{Zze^{2}}{r} - \frac{Zze^{2}}{b} \right) \right] dr} \right\}$$

$$= \exp \left\{ -\frac{2}{\hbar} \sqrt{(2mZze^{2})} \int_{R}^{b} \left(\frac{1}{r} - \frac{1}{b} \right)^{1/2} dr \right\} \qquad ... (i)$$

To evaluate the integral in (i), we put $r=b\cos^2\theta$. Then

$$\int \left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} dr = -2\sqrt{b} \int \sin^2 \theta \, d\theta = -\sqrt{b} \left(\frac{r}{b} - \frac{1}{2}\sin 2\theta\right)$$

$$= -\sqrt{b} \left[\cos^{-1} \sqrt{\left(\frac{r}{b}\right)} - \sqrt{\left(1 - \frac{r}{b}\right)} \cdot \sqrt{\left(\frac{r}{b}\right)}\right].$$

$$\therefore \int_{R}^{b} \left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} dr = \sqrt{b} \left[\cos^{-1} \sqrt{\left(\frac{R}{b}\right)} - \sqrt{\left(1 - \frac{R}{b}\right)} \sqrt{\frac{R}{b}}\right].$$
...(ii)

Let
$$\sqrt{\left(\frac{R}{b}\right)} = X << 1$$
, then

$$\cos^{-1} X \approx \left(\frac{\pi}{2} - X\right) \left\{ \because \cos\left(\frac{\pi}{2} - X\right) = \sin X \approx X \right\}$$

and $\cos^{-1} X - X (1 - X^2)^{1/2} \cong \frac{\pi}{2} - X - X (1 - X^2)^{1/2}$

$$\approx \frac{\pi}{2} \left(1 - \frac{4X}{\pi} \right)$$
. ...(iii)

$$\int_{R}^{b} \left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} dr = \sqrt{(b)} \cdot \frac{\pi}{2} \left\{ 1 - \frac{4}{\pi} \sqrt{\left(\frac{R}{b}\right)} \right\}. \quad \dots \text{(iv)}$$

The kinetic energy E is given by

$$\frac{1}{2}mv^2 = \frac{Zze^2}{b}$$

$$b = \frac{2Zze^2}{ze^2}.$$

or

as

Substituting this value of b into (iv), we get

$$\int_{R}^{b} \left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} dr = \frac{\pi}{2} \sqrt{\left(\frac{2Zze^2}{mv^2}\right)} \left[1 - \frac{4}{\pi} \sqrt{\left(\frac{Rmv^2}{2Zze^2}\right)}\right]$$

$$= \frac{\pi}{2} \sqrt{\left(\frac{4Ze^2}{mv^2}\right)} \left[1 - \frac{4}{\pi} \sqrt{\left(\frac{Rmv^2}{4Ze^2}\right)}\right]$$

$$(\because Z = 2 \text{ for } \alpha\text{-particle}).$$

Using this value into (i), we get the transmission probability

$$T^2 = \exp\left[-\frac{2}{\hbar}\left(\frac{2\pi Ze^2}{v} - 4e\sqrt{mZR}\right)\right]. \qquad ...(v)$$

If we assume that the α -particle inside the nucleus is moving backward and forward along a radius with velocity v, then it will collide at r=R; $\frac{v}{2R}$ times per sec, or the time taken for each collision is $\frac{2R}{n}$ secs. The probability of finding the α -particle outside the nucleus at r=b during each collision is given by expression (v). Hence the average life of the nucleus for α -decay will be

$$T_{0} = \frac{2R}{v} \cdot T^{2} = R \sqrt{\left(\frac{2m}{E}\right)} \cdot T^{2} \left\{ : v = \sqrt{\left(\frac{2E}{m}\right)} \operatorname{from} E = \frac{1}{2}mv^{2} \right\}$$

$$= R \sqrt{\left(\frac{2m}{E}\right)} \exp \left[-\frac{2}{\hbar} \left(\frac{2\pi Ze^{2}}{v} - 4e\sqrt{mZR}\right) \right] \cdot \dots (vi)$$

The half life That is given by the relation

$$T_{half} = .693 \Gamma_a$$
 ...(vii)

$$T_{half} = .693R \sqrt{\left(\frac{2m}{E}\right)} \exp \left[-\frac{2}{\hbar} \left(\frac{2\pi Ze^2}{v} - 4e\sqrt{(mZR)}\right)\right] \cdot ...(viii)$$

Problem 22. What is the spontaneous emission probability per unit time, expressed in sec-1, for a hydrogen atom in its first excited state?

Sol. The transition probability per unit time for the spontaneous emission is given by equation (203) as

$$A = \frac{4e^2\omega^3}{3\hbar c^3} |\langle k | \mathbf{r} | n \rangle|^2. \qquad \dots (i)$$

In the present case, k is the first excited state of hydrogen (2p-state) and n is the ground state of the hydrogen (ls-state), i.e.

$$|n\rangle = R_{1r}(r) Y_0^0(\theta, \phi), \text{ and}$$

$$|R_{2p}(r) Y_1^0(\theta, \phi);$$

$$|k\rangle = \begin{cases} R_{2p}(r) Y_1^1(\theta, \phi); \\ R_{2p}(r) Y_1^1(\theta, \phi), \\ R_{2p}(r) Y_1^{-1}(\theta, \phi). \end{cases}$$

There are three $|k\rangle$ states, and the transition probability for each of this is the same. Hence, we can calculate any one of them. Let us take $|k\rangle = R_{2p}(r) Y_1^0(\theta, \phi)$. Then

 $\frac{1}{3} |\langle k | r | n \rangle|^2 = |\langle k | x | n \rangle|^2 = |\langle k | y | n \rangle|^2 = |\langle k | z | n \rangle|^2$, because the states $|k\rangle$ and $|n\rangle$ are spherically symmetric. Now we evalute

we evalute
$$\langle k \mid z \mid n \rangle = \int R_{2p}(r) Y_1^{0*} r \cos \theta R_{1s}(r) Y_0^{0} r^2 dr d\Omega$$

$$= \int R_{2p}(r) Y_1^{0*} r \sqrt{\left(\frac{4\pi}{3}\right)} Y_1^{0} \cdot \frac{1}{\sqrt{(\pi a_0^3)}} e^{-r/a_0} r^2 dr d\Omega$$

$$= \int \left(\frac{4\pi}{3a_0^3}\right) \int_0^\infty R_{2p}(r) r^3 e^{-r/a_0} dr$$

$$\left\{ :: \int Y_1^{0*} Y_1^{0} d\Omega = 1 \right\}$$

$$= \sqrt{\left(\frac{4}{3a_0^{3}}\right)} \cdot \frac{1}{(2a_0)^{3/2}} \cdot \frac{1}{a_0\sqrt{(3)}} \int_0^\infty e^{-r/2a_0} e^{-r/a_0} dr$$

$$= \sqrt{\left(\frac{4}{3a_0^{3}}\right) \cdot \frac{1}{(2a_0)^{3/2}} \cdot \frac{1}{a_0\sqrt{(3)}} \cdot \frac{4!}{(\frac{3}{2}a_0)^5}} = \frac{2^3a_0}{3^5\sqrt{(2)}} \cdot \dots (ii)$$

$$\therefore |\langle k \mid r \mid n \rangle|^2 = 3 |\langle k \mid z \mid n \rangle|^2 = 3 \cdot \frac{2^{16}a_0^2}{3^{10} \cdot 2} \cdot \dots (iii)$$

Now, for the first excited state,

$$\hbar\omega \simeq 10.2 \text{ eV}$$
.

$$\omega \simeq \frac{10.2}{\hbar} \times 10^{-12} \text{ ergs} \simeq \frac{10^{-11}}{\hbar} \text{ ergs}.$$
Sing
$$c = 4.8 \times 10^{-10} \text{ e.s.u.}$$

Using,

$$e = 4.8 \times 10^{-10}$$
 e.s.u.,

$$\hbar \simeq 10^{-27}$$
 erg-sec.,

$$c \approx 10^{10}$$
 cm/sec.,

and

$$a_0 \cong 10^{-8} \text{ cms.},$$

into (i) along with the value (iii), we obtain

$$A \cong 10^{10} \text{ sec}^{-1}$$
.

...(ii)

From it, the life time of the first excited state of hydrogen atom will be

$$r \cong \frac{1}{A} = 10^{-10} \text{ secs.}$$
 ...(v)

The actual life time is 10^{-8} secs.

The study of scattering processes has been a very important field of physics. A knowledge of the properties of atomic and molecular collisions is of basic importance in many fields, such as properties of gases, the theory of chemical reactions and collision processes in astrophysics. In the atomic nuclei most of our present knowledge about nuclear interactions has come from the study of nuclear collission processes. Furthermore, even more important is the fact that from a detailed study of the results of scattering, much can be learnt about the nature of the particles that are being scattered as well as of those that are doing the scattering. In this chapter we shall consider the quantum mechanical treatment of the scattering of a particle by a potential, and the equivalent problem of the scattering of a particle with another particle. We shall be concerned mostly with approximate methods, which will be suitable for various circumstances.

In some of the collisions, the energy of incident particle does not change. Such collisions are called elastic collisions and such scattering is called the *elastic scattering*. When the energy of a particle is altered after its interaction with a potential or with another particle, the scattering is called *inelastic scattering*.

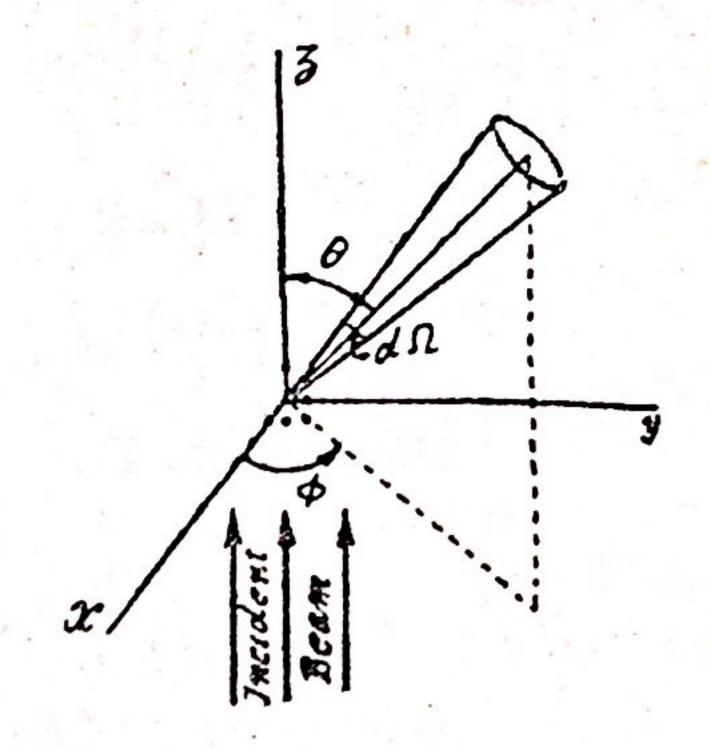
9.1 THE SCATTERING CROSS-SECTION:

Scattering cross-section is a quantity in terms of which we can describe the angular distribution of the particles scattered by a fixed centre of force or by some other particles.

Suppose, a mono energetic beam of particles is directed towards a scattering centre consisted of n number of scatterers which deflects or scatters the incident particles in various directions. The scattered particles diverge. Eventually, at large distances from the target (where they are detected by suitable instruments), their motion is directed radially outwards. Let us count the number of scattered particles per unit time in a small solid angle element $d\Omega$

centred about a direction that has polar angles θ and ϕ with res-

pect to bombarding direction as polar axis (see fig. 1) If N_s is the number of particles scattered in the solid angle $d\Omega = \sin \theta \ d\theta \ d\phi$ per second, then N_s will be proportional to the incident flux N (the number of particles crossing unit area taken normal to the heam direction per unit time), the number of scatteres 'n'; and the solid angle element $d\Omega$; i.e.,



 $N_s \propto Nn.d\Omega$

Fig 1.

The proportionality factor, which depends in general on θ and ϕ , is called the differential scattering cross-section, and is denoted by $\left(\frac{d\sigma}{d\Omega}\right)$. Therefore,

$$N_s = \frac{d\sigma (\theta, \phi)}{d\Omega} . N. n. d\Omega \qquad ...(1)$$

In order to find the dimensions of $\left(\frac{d\sigma}{d\Omega}\right)$, we see that the dimension of N_s is $\frac{1}{T}$, that of N is $\frac{1}{L^2T}$ and the number of scatterer 'n' and the solid angle Ω are dimensionless. Hence the dimensions of $\left(\frac{d\sigma}{d\Omega}\right)$ is given by

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{N_s}{N.n.d\Omega} = \frac{L^2T}{T} = L^2$$

Thus the dimensions of $\left(\frac{d\sigma}{d\Omega}\right)$ is that of the area, which

justifies the term 'cross-section'. It is interpreted as the area of incident beam through which the scattered particles in the solid angle $d\Omega$ passes. Differential scattering cross-section depends only on the parameters of the incident particle and the nature of the target, Given this information, the aim of scattering theory is to determine $\left(\frac{d\sigma}{d\Omega}\right)$ as a function of θ and ϕ . The total scattering cross-section σ_{tot} , may be obtained from it by integration over all directions.

$$\sigma_{tot} = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega = \int_0^{2\pi} \int_0^{\pi} \left(\frac{d\sigma}{d\Omega}\right) \sin\theta \, d\theta \, d\phi \, d\phi \qquad \dots (2)$$

In most of the cases we consider, $\left(\frac{d\sigma}{d\Omega}\right)$ as independent of ϕ . Then eqn. (2) simplifies to

$$\sigma_{tot} = 2\pi \int \left(\frac{d\sigma}{d\Omega}\right) \sin\theta \ d\theta \qquad ...(3)$$

In the above definition of the scattering cross-section, we have not taken into account the interaction among the incident particles and the effect due to multiple scattering. This is justified if the number of scatteres is very mall and the incident flux is large 9.2. LABORATORY AND CENTRE OF MASS SYSTEMS:

Scattering processes can be visualized in two types of coordinate system:

- (i) Laboratory System. In this co-ordinate system bombarded particle (or target) is initially at rest.
- (ii) Centre of Mass System. In this coordinte system, the centre of mass of two colliding particles is always at rest.

It is easier to calculate the results of collision experiments in the centre of mass system than that in the laboratory system; because there are three degrees of freedom in the centre of mass system as compared to six degree of freedom in the laboratory system. Usually we make the calculations in the centre of mass (C.M.) system and the observations are made in the laboratory (L) system. Therefore, it is necessary to establish a relationship between the two types of coordinate system

Ralation Between L and C.M. System:

Let a particle of mass m_1 and initial velocity v_1 strikes a particle of mass m_2 at rest in the L-sysem (fig. 2). Therefore, before collision, the centre of mass moves to the right with a velocity $v_{c\cdot m}$. Hence we have, from

the conservation of momentum, the

$$(m_1 + m_2) v_{c m} = m_1 v_1$$

$$v_{c m} = \frac{m_1}{m_1 + m_2} v_1$$

$$= \frac{m_1 m_2}{m_2 (m_1 + m_2)} v_1$$

$$= \frac{\mu}{m_1} v_1$$

$$= \frac{\mu}{m_2} v_1$$

$$= (4)$$
Fig. 2

or

where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass of the particles.

In the centre of mass system, the particle of mass m_1 approaches the centre of mass with a speed $(v_1-v_{c\cdot m})$; since the centre of mass in the C.M. system remains always at rest. The other particle will move with a speed $v_{c\cdot m}$ in the opposite direction (fig. 3).

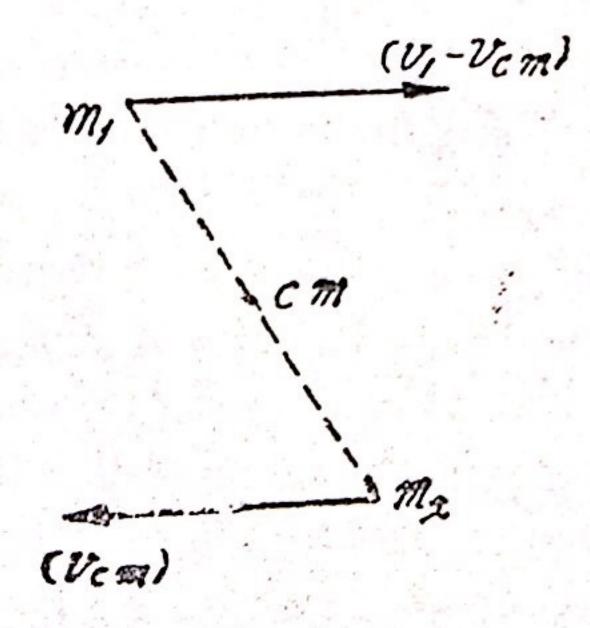


Fig. 3.

For elastic collisions, in which the speed does not change after the collision, the situation after the collision in the above two systems is show below in figs. 4 and 5; respectively.

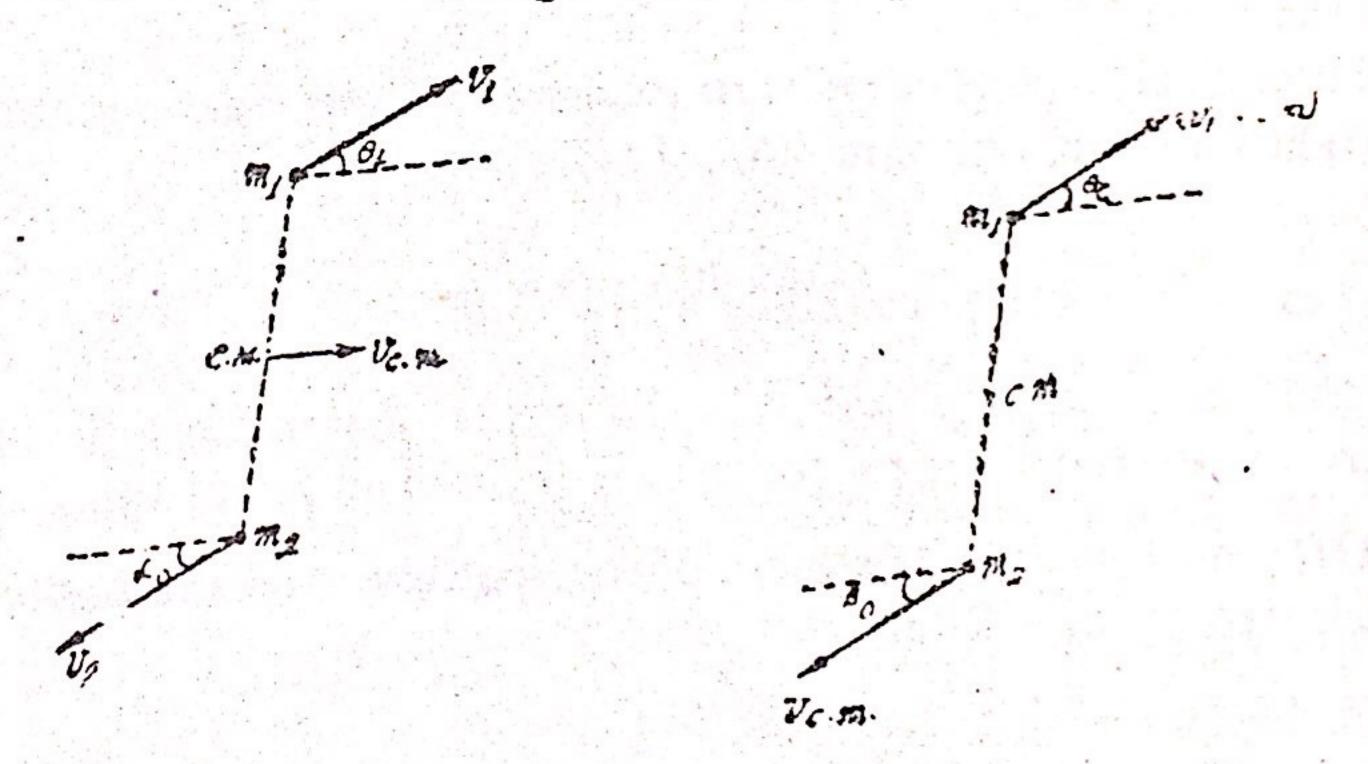


Fig. 4.

Fig. 5.

Now the vector sum of the final velocity of the particle in the C,M. system and the velocity of the centre of mass of the two particles in the L system gives the final velocity of the particle in the L system. (see fig. 6) From fig. 6 we have

$$\tan \theta_L = \frac{AB}{QA} = \frac{(v_1 - v_{c \cdot m \cdot}) \sin \theta_c}{v_{c \cdot m \cdot} + (v_1 - v_{c \cdot m \cdot}) \cos \theta_c}$$

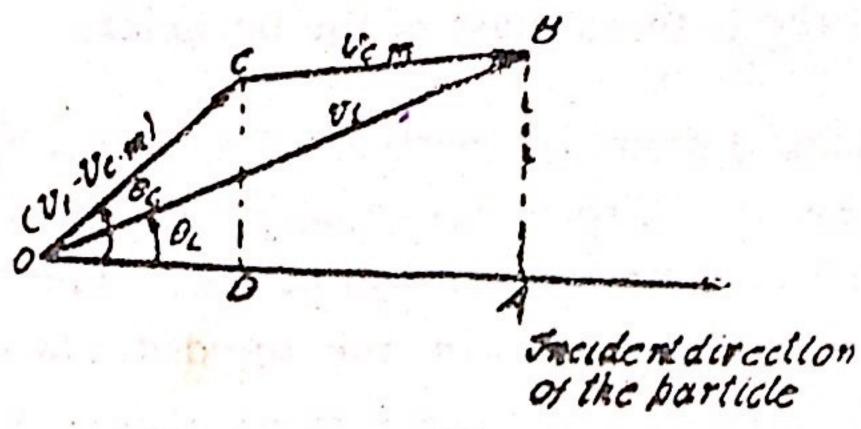


Fig. 6.

$$= \frac{\sin \theta_c}{\frac{v_{c \cdot m}}{v_1 - v_{c \cdot m}} + \cos \theta_c} \dots (5)$$

Further,
$$\frac{v_{c \cdot m}}{v_1 - v_{c \cdot m}} = \frac{m_1 v_1 / (m_1 + m_2)}{v_1 - m_1 v_1 / (m_1 + m_2)} = \frac{m_1}{m_2} = \gamma \text{ (say)}$$

$$\therefore \quad \tan \theta_L = \frac{\sin \theta_c}{\gamma + \cos \theta_c} \qquad \dots (6)$$

This gives the relationship between the angle of seattering in the L system and that in the C.M. system. We can discuss the following three cases:

(I) $m_2 \gg m_1$ i.e., the mass of the scatterer is much larger than the mass of the incident particle. Then $\gamma \ll 1$ and hence it can be neglected in comparision to $\cos \theta_c$ in the denominator of the right hand side of eqn. (6). Thus

$$\tan \theta_L = \frac{\sin \theta_c}{\cos \theta_c} = \tan \theta_c \Rightarrow \theta_L = \theta_c$$

i.e., the angle of scattering in both the system is the same. Electron scattered by a proton target is an example of this case.

(II) $m_1=m_2$, i.e., the mass of the scatterer and the scattered particle are equal. Then $\gamma=1$, and

$$\tan \theta_{L} = \frac{\sin \theta_{c}}{1 + \cos \theta_{c}} = \frac{2 \sin \frac{\theta_{c}}{2} \cos \frac{\theta_{c}}{2}}{1 + \cos^{2} \frac{\theta_{c}}{2} - \sin^{2} \frac{\theta_{c}}{2}}$$

$$= \frac{2 \sin \frac{\theta_{c}}{2} \cos \frac{\theta_{c}}{2}}{2 \cos^{2} \frac{\theta_{c}}{2}} = \tan \frac{\theta_{c}}{2} \Rightarrow \theta_{L} = \frac{\theta_{c}}{2}$$

In the case, the angle of scattering in the L system is half of the angle of scattering in C.M. system. Proton scattering by a proton target is an example of this case.

(III) $m_2 < m_1$, i.e. the mass of the scatterer is smaller than the mass of the scattered particle. In this case, θ_L first increases from zero to a maximum value $\sin^{-1}(1/\gamma)$, which is less than $\frac{\pi}{2}$, as θ_c increases from zero to $\cos^{-1}(1/\gamma)$. Then θ_L decreases to zero as θ_c increases further to π . These three cases are depicted pictorially in the fig. 7.

Now we shall find the relationship between the scattering cross sections in the L system and that in the C.M. system. This can be done by using equation (6). According to the scattering cross-section, same number of particles are scattered into the differential solid angle $d\Omega_L$ about (θ_L, ϕ_L) as are scattered into $d\Omega_c$ about (θ_c, ϕ_c) . Therefore,

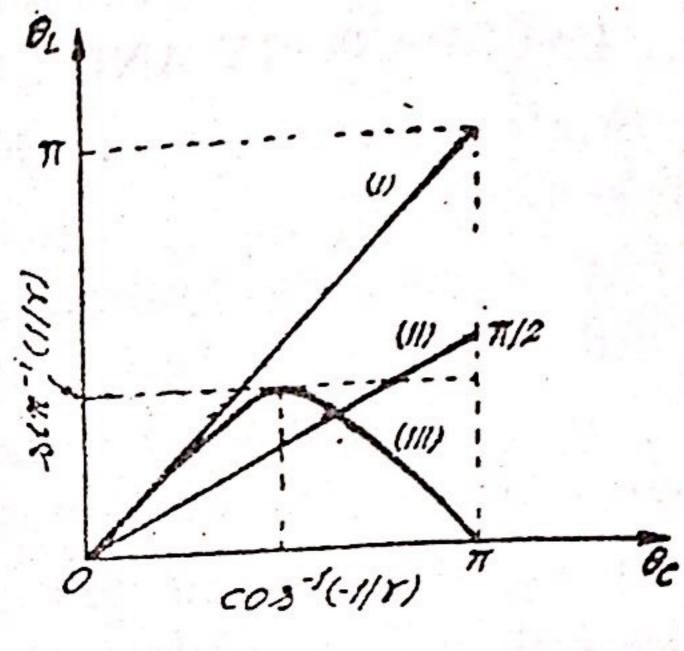


Fig. 7.

$$\sigma (\theta_L, \phi_L) d\Omega_L = \sigma (\theta_c, \phi_c) d\Omega_c$$

$$2\pi\sigma (\theta_L, \theta_L) \sin \theta_L d\theta_L = 2\pi \sigma (\theta_c, \phi_c) \sin \theta_c d\theta_c$$

$$\sigma (\theta_L, \phi_L) \sin \theta_L d\theta_L = \sigma (\theta_c, \phi_c) \sin \theta_c, d\theta_c \dots (7)$$

Differentiating eqn. (6) we get

$$\sec^{2} \theta_{L} d^{2}_{L} = \frac{(\cos \theta_{c} + \gamma) \cos \theta_{c} + \sin^{2} \theta_{c}}{(\gamma + \cos \theta_{c})^{2}} d\theta_{c}$$
$$= \frac{1 + \gamma \cos \theta_{c}}{(\gamma + \cos \theta_{c})^{2}} d\theta.$$

$$\sin \theta_L \ d\theta_L = \frac{\sin \theta_L}{\sec^2 \theta_L} \cdot \frac{1 + \gamma \cos \theta_c}{(\gamma + \cos \theta_c)^2} \ d\theta_c$$

From eqn. (6),

or

or

$$\sin \theta_L = \frac{\cos \theta_L}{\gamma + \cos \theta_c} \sin \theta_c = \frac{\sin \theta_c}{\sec^2 \theta_L (\gamma + \cos \theta_c)}$$

Hence we have,

$$\sin \theta_L d\theta_L = \frac{1 + \gamma \cos \theta_c}{\sec^3 \theta_L (\gamma + \cos \theta_c)^3} \sin \theta_c d\theta_c \dots (8)$$
Now,
$$\sec^3 \theta_L = (1 + \tan^2 \theta_L)^{3/2}$$

$$= \left(1 + \frac{\sin^2 \theta_c}{(\gamma + \cos \theta_c)^2}\right)^{3/2} = \left[\frac{(\gamma + \cos \theta_c)^2 + \sin^2 \theta_c}{(\gamma + \cos \theta_c)^2}\right]^{3/2}$$

$$=\frac{(1+2\gamma\cos\theta_c+\gamma^2)^{3/2}}{(\gamma+\cos\theta_c)^3}$$

Using it in (8) we obtain

$$\sin \theta_L d\theta_L = \frac{1 + \gamma \cos \theta_c}{(1 + 2\gamma \cos \theta_c + \gamma^2)^{3/2}} \cdot \sin \theta_c d\theta_c$$

Using it in (7), we get the relation between the scattering crosr-ection in the L system and that in the C.M. system as

$$\sigma(\theta_L, \phi_L) = \frac{(1+2\gamma \cos \theta_c + \gamma^2)^{3/2}}{1+\gamma \cos \theta_c} \sigma(\theta_c, \phi_c). \qquad ...(9)$$

9.3. ASYMPTOTIC BEHAVIOUR OF THE WAVE-FUNCTION

Let us consider the scattering of a beam of particles of fixed energy by a target at the origin. Since the energy of the particles is taken as fixed, there will be an infinite uncertainty in the measurement of time due to the Heisenberg's principle. Thus the system will be independent of time and we can describe it by the time independent Schroedinger equation

$$\left[\nabla^2 + k^2 - \frac{2m}{\hbar^2} V(\mathbf{r}) \right] \psi = 0 \qquad ...(10)$$

for the relative motion of the incident particle and the scatterer. Here m is the reduced mass of the incident particle and the scatterer, and $V(\mathbf{r})$ represents the interaction between the scattered particle and the scatterer. Differential scattering cross-section in the C.M. system can be found from the asymptotic form of the solution of eqn. (10). The boundary condition common to all scattering problems is that at large distances from the scattering region (or when the colliding particles are far apart) we want ψ to contain a part $\psi_{incident}$ that represents an incident particle moving in a particular direction, say along z-axis, and a part $\psi_{scatter}$ that represents a wave diverging from the scatterer (or a radially outgoing particle). In other words, we seek a solution of eqn. (10) which asymptotically represents an incoming plane wave (along the z-direction) and a spherical outgoing (scattered) wave. Thus

$$\psi \longrightarrow A \left[exp. (ikz) + f(\theta) \frac{exp. (ikr)}{r} \right] = \psi_{incident} + \psi_{scattered}, \dots (11)$$

Where θ is the angle of scattering; i.e., the angle between the direction of scattered wave and the original direction, and A is

the normalization constant. The angle ϕ and k do not appear because of the symmetry of V(r). In the region $r \to \infty$ ($V(r) \to 0$), eqn. (10) for $\psi_{scattered}$ becomes

 $(\nabla^2 + k^2) \psi_{scattered} = 0. \tag{12}$

when $\psi_{scattered} = f(\theta) \exp(ikr)/r$ is substituted into this equation, it is easily seen that the only term of the order 1/r in $\nabla^2 \psi_{scattered}$ is $k^2 \psi_{scattered}$; other terms are of higher order. Therefore, as required, (11) satisfies (10) asymptotically through terms of order 1/r in the region of interest $(\nu(r)=0)$ for any form of the function $f(\theta)$. The function $f(\theta)$ is called the scattering amplitude or angiedistribution factor.

The first term of (11) represents a particle moving in positive z-direction or along the polar axis $\theta=0$. The second term represents a particle that is moving radially outward, and the function $f(\theta)$ gives the angular dependence of its amplitude. To find the physical meaning of the coefficient of normalization A and the angular function $f(\theta)$, we see that the particle density for the incident wave is given by:

$$|\psi_{incident}|^2 = |A \exp_{\cdot}(ikz)|^2 = |A|^2$$

If v is the velocity of the incident particle, then the incident flux is equal to $v \mid A \mid^2$.

The particle density for the scattered wave is given by:

$$|\psi_{scattered}|^2 = |Af(r)| \frac{\exp[ikr]}{r} |^3 = |A|^2 \cdot |f(r)|^2$$

If we consider the elastic scattering, then the velocity of the scattered particle will be the same as that of the incident particle, and hence the scattered flux is equal to $v \mid A \mid^2 \cdot \mid f(\theta) \mid^2/r^2$.

Therefore the number of particles scattered per second into the solid angle $d\Omega = \sin \theta \, dt \, d$ is given by

$$N_{r} = |A|^{2} \frac{v}{r^{2}} |f(\theta)|^{2} ds$$

$$= |A|^{2} \frac{v}{r^{2}} |f(\theta)|^{2} r^{2} d\Omega$$

$$= |A|^{2} v |f(\theta)|^{2} d\Omega$$

Hence the differential scattering cross-section is given by:

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{N_s}{(\text{Incident Flux})d\Omega} = \frac{|A|^2 v |f(\theta)|^2 d\Omega}{|A|^2 v d\Omega}$$

$$= |f(\theta)|^2 \dots (13)$$

The total scattering cross-section is given by;

$$\sigma_{tot} = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega = \int |f(\theta)|^2 d\Omega \qquad \dots (14)$$

Thus, the choice of the coefficient A is unimportant as far as the calculation of the scattering cross section is concerned. The wavefunction may be normalized to unit incident flux by choosing $A=1/v^{1/2}$, or it may be normalized

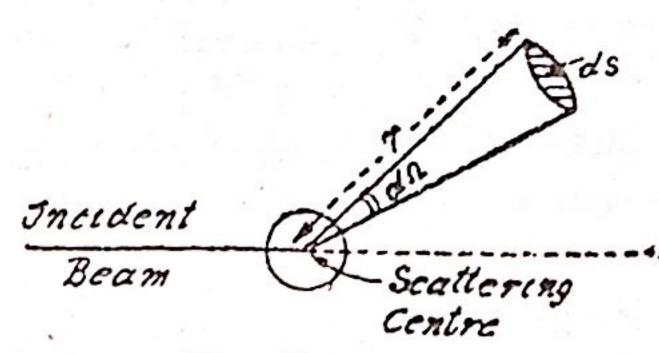


Fig (8)

by making $\int |\psi|^2 d^3r = 1$. We shall often simply set A = 1.

For inelastic scattering, velocities of the incident and the scattered particles are different. Let v_i be the velocity of the incident particle and v_s be that of the scattered particle. Then,

Incident flux =
$$v_i \mid A \mid^2$$

Scattered flux =
$$v_s \frac{|A|^2}{r^2} |f(\theta)|^2$$

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{v_i}{v_i} |f(\theta)|^2 \qquad \dots (15)$$

If k_i and k_s are the magnitudes of the propagation vectors for the incident and the scattered particles; respectively, then

$$\hbar k_i/m = v_i$$
 and $\hbar k_s/m = v_s$

Hence we have

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{k_s}{k_t} |f(\theta)|^2 \qquad \dots (16)$$

9.4. PARTIAL WAVE METHOD:

It has been seen that we need the behaviour of the wavefunction at large distances (asymptotic behaviour) in order to find the scattering cross-section. Thus we should find the solution of the Schrodinger equation

$$\left(-\nabla^2 + \frac{2m}{\hbar^2} V(\mathbf{r})\right) \psi(\mathbf{r}) = \frac{2mE}{\hbar^2} \psi(\mathbf{r}). \qquad \dots (17)$$

throughout all space. For it we assume that the potential V(r) is spherically symmetric, i.e., it is a function of r only. Thus the wave equation (17) can be separated into the radial part and the angular part. We shall find the connection between the solutions separated into spherical polar coordinates and the assymptotic form (11). The procedure is called the method of partial waves.

Solutions of (17) can be written in the form $R_i(r) Y_i^m (\theta, \phi)$, where the radial wave functions $R_i(r)$ satisfy the equation

"THEORY OF SCATTERING"

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + k^2 - U(r) - \frac{l(l+1)}{r^2}\right] R_l(r) = 0;$$
with
$$U(r) = \frac{2m}{\hbar^2} V(r), \text{ and } k^2 = \frac{2mE}{\hbar^2} \qquad ...(18)$$

The general solution of the Schroedinger equation can be written as a linear combination of such solutions. Since we are considering spherically asymmetric potential, the problem possesses symmetry about the polar axis and hence the solutions will be independent of the angle ϕ . Hence, only the function,

$$R_l(r) Y_l^0(\theta, \phi) \propto R_l(r) P_l(\cos \theta),$$

appears in the linear combination. Thus we can write

$$\psi(r,\theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos \theta) \qquad ...(19)$$

In order to find the asymptotic form of the solution (19), we should solve the radial equation (18) for $R_l(r)$ and find its behaviour for $r \to \infty$. For it we write equation (18) by taking

$$R_l(r) = \chi_l(r)/r$$
.

We obtain,

$$\left[\frac{d^2}{dr^2} + k^2 - U(r) - \frac{l(l+1)}{r^2}\right] X_l(r) = 0 \qquad ...(20)$$

In the asymptotic region, both U(r) and l terms in (20) are very small. On neglecting these in comparison with k^2 , we obtain the approximate asymptotic solutions $x_l(r) \propto \exp[\pm ikr]$. To improve this approximation, let us suppose that

$$X_l(r) = T_l(r) e^{\pm ikr}, \qquad \dots (21)$$

where $T_l(r)$ is expected to be very slowly varying in the asymptotic region. On introducing this into (20) we get;

$$\left[\frac{d^2}{dr^2} \pm 2ik \frac{d}{dr} - U(r) - \frac{l(l+1)}{r^2}\right] T_1(r) = 0 \qquad ...(22)$$

Since $T_l(r)$ varies very slowly at asymptotic distances, we can neglect its second derivative compared to its first derivative with respect to r. Hence, neglecting $\frac{d^2T_l(r)}{dr^2}$, solution of eqn. (22) is given by:

$$T_l(r) \simeq \exp\left[\pm \frac{1}{2ik} \int_0^r \left(U + \frac{l(l+1)}{r^2}\right) dr\right] \qquad ...(23)$$

For any potential decreasing faster than 1/r at infinity (i.e.

 $rU(r) \rightarrow 0$ as $r \rightarrow \infty$) the integral in eq. (23) is convergent, which means that if r is large enough, the value of the integral is effectively independent of r, and hence $T_l(r)$ will be constant in the asymptotic region. In the following, we will confine our attention to such potentials only. Then the asymptotic form of $\chi_l(r)$ is, in general, some linear combination of the two solutions $e^{\pm ikr}$ in eq. (21) with $T_l(r)$ constant. Without loss of generality, we can write any such combination in the form

$$\chi_i(r) \longrightarrow a_i \sin(kr + \delta_i')$$
 ...(24)

where a_i and δ_i are constants.

The boundary condition at the origin (r=0) requires that $R_l(r)$ should be finite. Thus $X_l(r)=r$ $R_l(r)$ should vanish at the origin. Since all quantities appearing in the differential eq. (20) for $X_l(r)$ are real, and $X_l(r)$ vanishes at the origin, it is easy to convince ourself that X_l must be real everywhere, apart from an overall factor which is arbitrary and may be complex. Thus δ_l in eq. (24) must be real, though a_l may be complex.

Let us now compare the above asymptotic behaviour with that of the partial waves for a free particle (U(r)=0). For U(r=0)=0 we can write eqn. (18) as

$$\begin{bmatrix} \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2} \end{bmatrix} R_l(r) = 0 \qquad \dots (25)$$

The general solution of this equation is a linear combination of the spherical Bessel functions $j_l(kr)$ and the spherical neumann functions $n_l(kr)$. The only admissible solution is $j_1(kr)$; because $n_l(kr)$ becomes infinite at r=0. Thus $R_l(r)=cj_l(kr)$, where c is a constant. Since the asymptotic forms of the spherical Bessel functions are known to be given by

$$\frac{j_{l}(kr) \xrightarrow{r \to \infty} \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right)}{n_{l}(kr) \xrightarrow{r \to \infty} \frac{-1}{kr} \cos\left(kr - \frac{l\pi}{2}\right)} \dots (26)$$

it follows that $\chi_l(r) = r R_l(r) \xrightarrow{} c \sin(kr - l\pi/2)$. Hence in

this case, χ_l has the asymptotic form (24) with $\delta_l' = -\frac{1}{2}l\pi$. Thus the effect of the potential on the partial waves in the asymptotic region is simply to change the phase from $-\frac{1}{2}\pi l$ to some other value δ_l' . This change,

$$\delta_l = \delta_l' + \frac{1}{2}l\pi \qquad ...(27)$$

is called the phase shift in the 1th partial wave. Since δ_l is real, δ_l is also real.

From (24) and (27), the asymptotic form of $R_l(r)$ is given by $R_l(r) \xrightarrow[r \to \infty]{A_l} \sin(kr - \frac{1}{2}l\pi + \delta_l)$

where $A_i = ka_i$. Hence the asymptotic form of $\psi(\mathbf{r})$ is given by

$$\psi(\mathbf{r}) \xrightarrow{r \to \infty} \sum_{l} \frac{A_{l}}{kr} \sin(kr - \frac{1}{2}l\pi + \delta_{l}) P_{l}(\cos\theta) \dots (28)$$

We have to choose A_l in such a way that this form agrees with the form (11); given by

$$\psi(\mathbf{r}) \xrightarrow[r \to \infty]{} e^{ikz} + \frac{f(\theta)}{r} e^{ikr} \qquad ...(29)$$

For it we need the following expansion:

$$e^{ikz}$$
 = exp. $(ikr \cos \theta) = \sum_{l=0}^{\infty} (2l+1) i^l j_l (kr) P_l (\cos \theta)$

$$\frac{1}{r \to \infty} \sum_{l=0}^{\infty} (2l+1) i^{l} (kr)^{-1} \sin (kr - \frac{1}{2}l\pi) P_{l} (\cos \theta) \dots (30)$$

Substituting (30) into (29) we get:

$$\psi(\mathbf{r}) \xrightarrow[r \to \infty]{\infty} \sum_{l=0}^{\infty} (2l+1) i^{l} \frac{\sin(kr-l\pi/2)}{kr} P_{l}(\cos\theta) + \frac{f(\theta)}{r} e^{ikr} \dots (31)$$

Both the equations (31) and (28) are the same. Thus, when we write sine functions in complex exponential form, the coefficients of e^{ikr} and that of e^{-ikr} should be equal in both the equations.

Comparing the co-efficients of eikr we get:

$$\sum_{l=0}^{\infty} \frac{A_l}{2ikr} P_l (\cos \theta) \exp \left[i \left(\delta_l - \frac{l\pi}{2} \right) \right]$$

$$= \sum_{l=0}^{\infty} (2l+1) i^{l} P_{l} (\cos \theta) \frac{e^{il\pi 2}}{2ikr} + \frac{f(\theta)}{r} ...(32)$$

and on equating the coefficients of e^{-ikr} , we have

$$\sum_{l=0}^{\infty} \frac{A_{l}}{2ikr} \exp \left[-i\left(\delta_{l} - \frac{l\pi}{2}\right)\right] P_{l} \left(\cos\theta\right)$$

$$= \sum_{l=0}^{\infty} \frac{(2l+1)}{2ikr} i^{l} P_{l} (\cos \theta) \exp \left(i l \frac{\pi}{2}\right) ...(33)$$

From it we have,

$$A_l = (2l+1) i^l \exp_{-1}(i\delta_l)$$

Using this value in (32):

$$\sum_{l=0}^{\infty} (2l+1) i^{l} \frac{\exp. (i\delta_{l})}{2ikr} \exp. \left[i \left(\delta_{l} - l\pi/2\right)\right] P_{l} \left(\cos \theta\right)$$

$$= \sum_{l=0}^{\infty} (2l+1) i^{2} \frac{\exp(-i l\pi/2)}{2ikr} P_{l} (\cos \theta) + \frac{f(\theta)}{r}$$

From it, we have

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) i^{l} \exp. (-il \pi/2) \{ \exp. (2i\delta_{l}) - 1 \} P_{l} (\cos \theta)$$

or
$$f(\theta) \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \{ \exp. (2i\delta_l) - 1 \} P_l (\cos \theta)$$
 ...(34)

$$\{i^l = e^{il\pi/2}\}$$

We can write (34) in a slightly modified form as:

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp \left\{i \delta_l\right\} \left[\frac{\exp \left\{i \delta_l\right\} - \exp \left\{-i \delta_l\right\}}{2i}\right] P_i \left(\cos \theta\right)$$

or
$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp_{l} \{i \delta_{l}\} \sin \delta_{l} P_{l} (\cos \theta)$$
 ...(35)

Using (13), we obtain the differential scattering cross-section as:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1) P_l (\cos \theta) \exp. \{i \delta_l\} \sin \delta_l \right|^2 \dots (36)$$

Using the orthonormality relation for the Legendre's polynomial,

$$\int P_{l}(\cos\theta) P_{l'}(\cos\theta) \sin\theta d\theta = \frac{2}{(2l+1)} \delta_{l'}$$

we get the total scattering cross-section as:

$$\sigma_{tot} = 2\pi \int_0^{\pi} \left(\frac{d\sigma}{d\Omega}\right) \sin \theta \, d\theta = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l \qquad \dots (37)$$

Optical Theorem. The optical theorem relates the total scattering cross-section to the scattering amplitude in the forward direction i.e. the scattering amplitude for $\theta=0$. Taking $\theta=0$ in eqn. (35) we get

$$f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp_{l} \{i \delta_{l}\} \sin \delta_{l}$$

$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) (\cos \delta_{l} + i \sin \delta_{l}) \sin \delta_{l}$$

$$I_{m}. f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^{2} \delta_{l} \qquad ...(38)$$

Comparing it with eqn. (37) we can write:

$$\sigma_{tot.} = \frac{4\pi}{k^-} I_m. f(\theta = 0).$$
 ...(39)

This relation is called the *optical theorem*. This shows that the imaginary part of the forward scattering amplitude measures the loss of intensity which the incident beam suffers because of the scattering. Thus the total scattering, cross-section represents the removal of flux from the incident beam, so that its intensity is smaller behind the scattering region $(\theta=0)$ than that in front of it. This is analogous to the optical shadow behind an obstacle and hence the above relation is called the optical theorem.

Phase Shifts: Relation to the Potential. From the asymptotic behaviour of the radial wave function $\chi_l(r)$:

$$\chi_{l}(r) \xrightarrow{r \to \infty} \frac{A_{l}}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_{l}\right) \qquad \dots (40)$$

we see that the phase shift δ_i is the difference between the phases of asymptotic from of the actual radial function $\chi_i(r)$ and the field free asymptotic solution $\chi_i^{(0)}(r)$. Field free solution $\chi_i^{(0)}(r)$ satisfies the equation.

$$\frac{d^2 \chi_i^{(0)}(r)}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2} \right] \chi_i^{(0)}(r) = 0, \qquad \dots (41)$$

and it is given by:

$$\chi_{l}^{(0)}(r) = r j_{l}(kr) \xrightarrow{r \to \infty} \frac{1}{k} \sin(kr - l\pi/2)$$
 ...(42)

Obviously, δ_l depends on the potential V(r). To obtain a rotation for δ_l in terms of V(r), we write from eqn. (20) an. (41) that

$$\int_{0}^{\infty} \left(\chi_{l}^{(0)} \frac{d^{2} \chi_{l}}{dr^{2}} - \chi_{l} \frac{d^{2} \chi_{l}^{(0)}}{dr^{2}} \right) dr = \int_{0}^{\infty} \chi_{l}^{(0)} U(r) \chi_{l} dr$$

or
$$\left[\chi_{l}^{(0)} \frac{d\chi_{l}}{dr} - \chi_{l} \frac{d \chi_{l}^{(0)}}{dr} \right]_{0}^{\infty} = \int_{0}^{\infty} \chi_{l}^{(0)} U(r) \chi_{l} dr \qquad ...(43)$$

Using eqns. (40) and (42), we obtain the following exact relation between δ_l and the potential V(r):

$$\sin \delta_{l} = -\int_{0}^{\infty} \sqrt{\left(\frac{\pi kr}{2}\right)} j_{l+1/2}(kr) U(r) \chi_{l}(r) dr ...(44)$$

In this equation $\chi_l(r)$ is the solution of eqn. (20). Function $\chi_l(r)$ is bounded at the origin (r=0), and it is normalized in such a way that for asymptotically large r,

$$\chi_{l}(r) \xrightarrow[r \to \infty]{} \frac{1}{k} \sin\left(kr - \frac{l\pi}{2} + \delta_{l}\right)$$

The expression (44) for the phase shift is purely formal inasmuch as we do not know $\chi_l(r)$ for all r. Nevertheless, it is useful as a starting point for approximate evaluation. Suppose, for instance, that $\chi_l(r)$ differs very little from $\chi_l^{(0)}$. Then,

$$\sin \delta_{l} = -\int_{0}^{\infty} \int \left(\frac{\pi kr}{2}\right) j_{l+1/2}(kr) U(r) \chi_{l}^{(0)}(r) dr \dots (45)$$
This is $1/2$

This is known as the Born approximation for phase shifts.

From eqns. (20) and (41), it is seen that for an attractive field χ_I is shifted inward relative to $\chi_I^{(0)}$, and for a repulsive field χ_I is shifted outward relative to $\chi_I^{(0)}$, i.e.

 $\delta_i > 0$ for attractive field $\delta_i < 0$ for repulsive field

Phase Shifts: Relation to the Energy. In fig. (9) we

show the plot of the function $R_l(r)$. The first and the largest maximum of $R_l(r)$ lies roughly at $r_{m:x}=l/k$. If the range a of the scattering potential is greater than r_{max} , then $R_l(r)$ will be quite large where the potential is also appreciable. Hence, there will be a strong interaction of the wave with the potential and a large phase shift

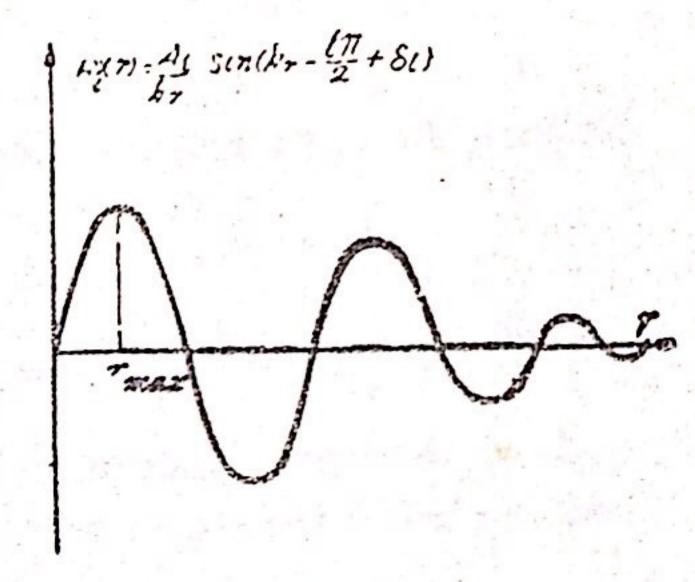


Fig. 9

will be introduced. On the other hand, if $r_{max} > a$, then $R_l(r)$ will be small where V(r) is appreciable. Thus, there will be very weak interaction of the wave with the potential and it will hardly be affected by the potential. Hence δ_l will be very small and the contribution to the scattering from this value of l will be negligible. So we conclude that the contribution to the scattering process comes only from the values of l which satisfy the condition.

$$a > r_{max} = \frac{1}{k}$$
or
$$l < ka; \qquad ...(46)$$

where a is the range of interaction of the potential. Hence we need not consider all the infinite number of phase shifts δ_l (l=0, 1, 2, ...). We have to consider the values of l from 0 to a maximum of the order of ka. Thus the expression (37) for the total scattering cross-section can be written as:

$$\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{ka} (2l+1) \sin^2 \delta_l \qquad ...(47)$$

We shall shortly see that the calculations for the phase shifts

 δ_l is a very cumbersome process. Hence smaller the magnitude of ka, easier is the partial wave method to apply. Thus the method of partial waves is most useful at low bombarding energies (small k) and small range (a) potentials. We have also seen that for the validity of this method, potential should be spherically symmetric and should fall off faster than 1/r. For large values of k and a, this method is very inconvenient. When ka << 1, only s-wave (l=0) are scattered. For ka=1, s(l=0) and p(l=1)? waves are scattered, and for other higher values of ka, the d(l=2), f(l=3), etc. waves also contribute in the scattering.

Calculation of δ_i 's. We make the calculation of the phase shifts δ_i for a potential of finite width 'a'.

$$V(r) = \begin{cases} V(r) & \text{for } 0 < r \le a \\ 0 & \text{for } r > a \end{cases}$$
 ...(48)

Since $U(r) = \frac{2m V(r)}{\hbar} = 0$ for r > a, in the exterior region

(r > a) the wave function must be a linear combination of $j_i(kr)$ and $n_i(kr)$. Thus we write

$$R_{l} = a_{l} j_{l} (kr) + b_{l} n_{l} (kr)$$

$$= A_{l} \left[\cos \delta_{l} j_{l} (kr) - \sin \delta_{l} n_{l} (kr)\right] \dots (49)$$

where we have put $a_l = A_l \cos \delta_l$ and $b_l = -A_l \sin \delta_l$. In this form we get the exact asymptotic form of $R_l(r)$ as:

$$R_{l}(r) \xrightarrow{r \to \infty} A_{l} \left[\cos \delta_{l} \frac{\sin (kr - l\pi/2)}{kr} + \sin \delta_{l} \frac{\cos (kr - l\pi/2)}{kr} \right]$$

$$= \frac{A_{l}}{kr} \sin \left(kr - \frac{l\pi}{2} + \delta_{l} \right)$$

We do not know R_l in the interior region (r < a), but we know from the boundary conditions that it has to match with the exterior wave function at r=a. In particular, if

$$\left. \frac{1}{R_l} \frac{dR_l}{dr} \right|_{r \to a-} = \beta_l$$

in the interior region, then $\frac{1}{R_l} \frac{dR_l}{dr}$ must also tend to β_l as $r \to a+$ in the exterior region.

From (49) we have

$$\beta_{l} = \frac{a}{R_{l}} \frac{dR_{l}}{dr} \bigg|_{r \to a+} = \left\{ \frac{ka \left[\cos \delta_{l} j_{l}' \left(kr \right) - \sin \delta_{l} n_{l}' \left(kr \right) \right]}{\cos \delta_{l} j_{l} \left(kr \right) - \sin \delta_{l} n_{l} \left(kr \right)} \right]_{r=a}$$

$$\therefore \beta_{l} \left[\frac{e^{i\delta l} + e^{-i\delta l}}{2} j_{l}(ka) - \frac{e^{i\delta l} - e^{-i\delta l}}{2i} n_{l}(ka) \right]$$

$$= ka \left[\frac{e^{i\delta l} + e^{-i\delta l}}{2} j_{l}'(ka) - \frac{e^{i\delta l} - e^{-i\delta l}}{2i} n_{l}'(ka) \right]$$
or $e^{i\cdot l} \left[\beta_{l} j_{l} + i\beta_{l} n_{l} - kaj_{l}' - ika n_{l}' \right] = e^{-i\delta l} \left[ka j_{l}' - ika n_{l}' - \beta_{l} j_{l} + i\beta_{l} n_{l} \right]$

or

$$e^{2i\delta l} = \frac{\beta_{l} (-j_{l} + in_{l}) + ka (j_{l}' - in_{l}')}{\beta_{l} (j_{l} + in_{l}) - ka (j_{l}' + in_{l}')}$$

$$= \frac{-(j_{l} - in_{l}) \left[\beta_{l} - ka \frac{j_{l}' - in_{l}'}{j_{l} - in_{l}} \right]}{(j_{l} - in_{l}) \left[\beta_{l} - ka \frac{j_{l}' + in_{l}'}{j_{l} + in_{l}} \right]} ...(50)$$

$$Now \qquad \frac{j_{l}' - in_{l}'}{j_{l} + in_{l}} = \frac{(j_{l}' - in_{l}')}{(j_{l} - in_{l})} + \frac{(j_{l} + in_{l})}{(j_{l} + in_{l})}$$

$$= \frac{j_{l}' j_{l} + n_{l}'n_{l} + i (j_{l}'n_{l} - n_{l}' j_{l})}{j_{l}^{2} + n_{l}^{2}}$$

Similarly,

$$\frac{j_{1}'+in_{1}'}{j_{1}+in_{1}} = \frac{j_{1}'j_{1}+n_{1}'n_{1}-i(j_{1}'n_{1}-n_{1}j_{1})}{j_{1}^{2}+n_{1}^{2}}$$

Using these expressions into (50) we get:

$$e^{2i\delta l} = -\frac{j_{l} - in_{l}}{j_{l} + in_{l}} \cdot \frac{\beta_{l} - ka \frac{j_{l}'j_{l} + n_{l}'n_{l} + i (j_{l}'n_{l} - n_{l}'j_{l})}{j_{l}^{2} + n_{l}^{2}}}{\beta_{l} - ka \frac{j_{l}'j_{l} + n_{l}'n_{l} - i (j_{l}'n_{l} - n_{l}'j_{l})}{(j_{l}^{2} + n_{l}^{2})}} \dots (51)$$

Making the substitutions,

$$ka\frac{j_{i}'j_{i}+n_{i}'n_{i}}{j_{i}^{2}+n_{i}^{2}}=\Delta_{1};-ka\frac{j_{i}'n_{i}'-n_{i}j}{j_{i}^{2}+n_{i}^{2}}=\frac{1}{ka(j_{i}^{2}+n_{i}^{2})}=S_{i},$$

and
$$-\frac{j_i-in_l}{j_i+in_l}=e^{2i\xi l}$$
, we can write (51) as:

$$e^{2i\delta l} = e^{2i\zeta l} \frac{\beta_l - \Delta_l + i S_l}{\beta_l - \Delta_l - i S_l} \dots (52)$$

Defining,

$$\tan \tau_{l} = \frac{S_{l}}{\beta_{l} - \Delta_{l}} \quad \text{or} \quad e^{2i\tau_{l}} = \frac{\beta_{l} - \Delta_{l} + iS_{l}}{\beta_{l} - \Delta_{l} - iS_{l}}, \text{ we have}$$

$$e^{2i\delta l} = e^{2i\xi l} e^{2i\tau^{l}}$$

$$\Rightarrow \delta_{l} = \xi_{l} + \tau_{l} \qquad ...(53)$$

Thus we see that the phase shift de for the 1th partial wave is consisted of two parts. The first part & given in terms of the

functions j_i and n_i of the field free radial equation and hence it is independent of the potential. The second part τ_i clearly depends upon the potential through the logrithmic derivative β_i .

Eq. (53) is a general expression for the phase shifts in terms of the known quantities. In practice we have to calculate the phase shifts in the low energy limit for which the partial wave method is most suitable. Hence we now consider the behaviour of the phase shift calculations for low incident energies. At low incidents energie, k will be very-very small and hence ka < < 1: i.e., only l=0 partial wave will contribute. Now, the beaviour of j_l and n_l near the origin is given by:

$$j_l(x) \xrightarrow[x \to 0]{} \frac{x^l}{(2l+1)!!}$$
 and $n_l(x) \xrightarrow[x \to 0]{} -\frac{(2l-1)!!*}{x^{l+1}}$

Therefore, for small values of k we can write:

$$\tan \xi_{l} = \frac{i_{l}(ka)}{n_{l}(ka)} \rightarrow -\frac{(ka)^{l}(ka)^{l+1}}{(2l+1)!!(2l-1)!!},$$

which is very small and hence we can replace $\tan \xi$, by ξ_i . Also, we have

$$S_{1} = \frac{1}{ka(j_{1}^{2} + n_{1}^{2})} \frac{1}{\text{small } k} \frac{1}{ka} \frac{1}{n_{1}^{2}} \xrightarrow{ka} \frac{(ka)^{2(l+1)}}{[(2l-1)!!]^{2}}$$

$$= \frac{(ka)^{2l+1}}{[(2l-1)!!]^{2}}$$

where we have neglected $j_l \xrightarrow{k \to 0} \frac{(ka)^l}{(2l-1)!!}$ compared to

$$m_1 \xrightarrow{k \to 0} -\frac{(2l-1)!!}{(ka)^{l+1}}$$
 for small values of ka . Lastly,

$$\therefore \tan \tau \cong \frac{(ka)^{2l+1}}{[(2l-1)!!]^2} \cdot \frac{1}{\beta_l + (l+1)},$$

is vevry small for ka < < 1, and hence we can replace $\tan \tau_i$ by τ_i .

Using the above approximations, the value of the phase shift at low incident energy is given by:

*
$$(2l+1)!! = 1.3, 5...(2l+1)$$

 $(2l-1)!! = 1.3, 5...(2l-1),$

$$\delta_{l} = \tau_{l} + \xi_{l} = \frac{(ka)^{2l+1}}{[(2l-1)!!]^{2}} \frac{(ka)^{2l+1}}{(\beta_{l}+l+1)} \frac{(ka)^{2l+1}}{(2l+1)!!} \left[\frac{(2l+1)!!}{(2l-1)!!} \frac{(2l+1)!!}{(2l-1)!!} \frac{1}{(2l-1)!!} \frac{(2l+1)!!}{(2l-1)!!} \frac{1}{(2l-1)!!} \frac{1}{(2l+1)!!} \frac{2l+1}{\beta_{l}+l+1} - 1 \right]$$

$$= \frac{(ka)^{2l+1}}{(2l+1)!!} \frac{1}{(2l-1)!!} \frac{1}{\beta_{l}+l+1} \frac{1}{\beta_{l}+l+1} \dots (54)$$

Thus, for small values of k we have

$$\delta_{l} \propto k^{2l+1} \qquad \dots (55)$$

This gives the energy dependence of the *l*th partial wave phase shit, δ_i ; when the incident energy is very small.

9.5. SCATTERING LENGTH AND EFFECTIVE-RANGE APPROXIMATION FOR SCATTERING OF SLOW PARTICLES:

It has been said that for low energy scattering, only s-wave (l=0) contribute in the scattering process. The scattering cross-section for slow particles can be written from eqn. (47) as:

$$\sigma_{tot} = \frac{4\pi}{k^2} \sin^2 \delta_0 \qquad \dots (56)$$

It is found that for low energy particles this can be described, instead of by δ_0 by two quantities which depend only on the range and the depth of the potential V(r), and not on its actual shape.

For s-wave, the Schroedinger equation (20) becomes

$$\frac{d^2\chi}{dr^2} + [k^2 - U(r)] \chi(r) = 0, \qquad U(r) = \frac{2m}{\hbar^2} V(r) \qquad ...(57)$$

Let $\chi_1(r)$ and $\chi_2(r)$ be the solutions for two energies k_1^2 , and k_2^2 . They satisfy the conditions

$$\chi_1(0) = 0, \chi_2(0) = 0;$$
 ...(58)

and we choose the normalization constanst in such a way that their asymptotic behaviour is given by

$$\chi_{1}(r) \xrightarrow{r \to \infty} \frac{1}{\sin \delta_{1}} \sin (k_{1} r + \delta_{1})$$

$$\chi_{2}(r) \xrightarrow{r \to \infty} \frac{1}{\sin \delta_{2}} \sin (k_{2} r + \delta_{2})$$
...(59)

Now, multiplying the equation for χ_1 by χ_2 and that for χ_2 by χ_1 and then subtracting from the first one, we get

$$\frac{d}{dr} \left[\chi_2 \frac{d\chi_1}{dr} - \chi_1 \frac{d\chi_2}{dr} \right] = (k_2^2 - k_1^2) \chi_1 \chi_2.$$

Integrating it from 0 to ∞ we obtain:

$$\left[\chi^{2} \frac{d\chi_{1}}{dr} - \chi_{1} \frac{d\chi_{2}}{dr}\right]_{0}^{\infty} = (k_{2}^{2} - k_{1}^{2}) \int_{0}^{\infty} \chi_{1} \chi_{2} dr \qquad \dots (60)$$

Let us consider two free particle (V(r)=0) solutions,

$$\phi_{1}(r) = \frac{1}{\sin \delta_{1}} \sin (k_{1} r + \delta_{1})$$

$$\phi_{2}(r) = \frac{1}{\sin \delta_{2}} \sin (k_{2} r + \delta_{2})$$
...(61)

which satisfy the equation.

$$\frac{d^2\phi}{dr^2} + k^2 \phi(r) = 0, \qquad ...(62)$$

with $k^2 = k_1^2$ and k_2^2 ; respectively. Then similar to eqn. (60), we here obtain:

$$\left[\begin{array}{c} \phi_2 \frac{d\phi_1}{dr} - \phi_1 \frac{d\phi_2}{dr} \right]_0^{\infty} = (k_2^2 - k_1^2) \int_0^{\infty} \phi_1 \, \phi_2 \, dr \qquad \dots (63)$$

On substracting eqn. (60) from (63), and using eqn. (58), (59) and (61) we get:

$$k_2 \cot \delta_2 - k_1 \cot \delta_1 = (k_2^2 - k_1^2) \int_0^\infty (\phi_1 \phi_2 - \chi_1 \chi_2) dr$$
 ...(64)
Defining the scattering level G

Defining the scattering length C_0 by:

$$-\frac{1}{C_0} = \lim_{k \to 0} [k \cot \delta(k)], \qquad ... (65)$$

we can write eqns. (64), on letting $k_1 \rightarrow 0$ and denoting k_2 by k,

$$k \cot \delta(k) = -\frac{1}{C_0} + k^2 \int_0^\infty (\phi_0 \phi - \chi_0 \chi) dr \qquad ...(66)$$

From eqns. (59), and (61), it is seen that the integrand in the eqn. differs from zero only in the region where U(r) is appreciable. In this region, the wavefunction $\chi(r)$ will not depend very much on the energy k^2 if |U(r)| is $\gg k^2$. We shall, therefore, make the approximation of replacing χ , ϕ by χ_0 , ϕ_0 ; the zero energy solutions. Thus from eqn. (66) we get

$$k \cot \delta(k) = -\frac{1}{C_0} + \frac{r_0}{2} k^2$$
 ...(67)

where,

$$r_0 = 2 \int_0^\infty (\phi_0^2 - \chi_0^2) dr$$

is called as the effective range of the potential V(r); and eqn. (67)

It is clear that both r_0 and C_0 are determined by U(r), and they are insensitive to the exact form of U(r) but depend only on some "integrated" or "average" property of U(r). From eqns. (59) and (61), it is seen that $(\phi_0^2 - X_0^2)$ and hence r_0 vanishes outside the "range" of U(r). If 'a' is the range of the potential, then the integral in (68) extends only to the radius a. The function ϕ_0 is a straight line from 1 at r=0, crossing the abscissa at $r=C_0$; X_0 is equal to it for r>a but bends down to zero at r=0. Hence we expect the r_0 to have a value roughly equal to $C(2, L_0)$, had the range of the potential. It is why we call r_0 as the effective range of the potential.

The effective range approximation is particularly useful when the potential is strong, because we expect the integral in (68) to be rather insensitive to k until the energy approaches a value comparable with the potential strength. Hence (67) can be expected to be a good approximation for the slow particles for which the energies are small compared with the potential strength. For this reason the effective-range formula has been especially useful in neutron proton scattering.

9.6. LEVINSON'S THEOREM:

This theorem gives a general qualitative information on the shape of the phase shift in the low energy domain. For simplicity, we resort to the square well potential

$$V(r) = \begin{cases} -V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases} \dots (69)$$

Now the Schroedinger equation can be solved easily. Inside the potential will we have:

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{2mV_0}{\hbar^2} + k^2 - \frac{l(l+1)}{r^2}\right]R_l(r) = 0 \qquad ...(70)$$

Putting
$$\alpha^2 = \left(k^2 + \frac{2mV_0}{\hbar^2}\right)$$
 it can be written as
$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \alpha^2 - \frac{l(l+1)}{r^2}\right]R_l(r) = 0 \qquad ...(71)$$

This equation is analogous to the free particle equation (25), and hence

$$R_1(r) = a_1 j_1(\alpha r) \text{ for } r < a$$
 ...(72)

Outside the potential, $R_l(r)$ is given by (49).

$$\therefore \beta_{l} = \frac{a}{R_{l}(r)} \cdot \frac{dR_{l}(r)}{dr} \Big|_{r \to a} = \frac{\alpha a j_{l}'(\alpha a)}{j_{l}(\alpha a)} \qquad ...(73)$$

In the low energy limit $(ka \le 1)$ only s-wave (l=0) contribute. Hence we have

$$\beta_0 = \alpha a \frac{j'_0(\alpha a)}{j_0(\alpha a)} = \frac{\alpha a}{\alpha a} \left[\alpha, a \cot \alpha, a - 1 \right] = \left[\alpha a \cot \alpha, a - 1 \right] \dots (74)$$

$$\left\{ \therefore j_0(x) = \frac{\sin x}{x} \text{ and } j'_0(x) = \frac{1}{x} \cos x - \frac{\sin x}{x^2} \right\}$$

We have seen that for low energy, $\nabla_i = -(l+1)$. Therefore, $\nabla_0 = -1$...(75)

Also, $S_l = \frac{(ka)^{2l+1}}{[(2l-1)!!]^2}$ gives

$$S_0 = ka \tag{76}$$

and

$$\xi_{l} = -\frac{(ka)^{l} (ka)^{l+1}}{(2l+1)!! (2l-1)!!} \Rightarrow \xi_{0} = -ka$$
 ...(77)

From eqns. (75), (76) and (77) we have,

$$\tan \tau_0 = \frac{S_0}{\beta_0 - \nabla_0} = \frac{ka}{\alpha a \cot \alpha a} = \frac{k}{\alpha} \tan \alpha a$$

or

$$\tau_0 = \tan^{-1}\left(\frac{k}{\alpha} \tan \alpha a\right) \qquad \dots (78)$$

$$\therefore \delta_0 = \tau_0 + \xi_0 = \tan^{-1} \left(\frac{k}{\alpha} \tan \alpha a \right) - ka \qquad \dots (79)$$

From (79) we see that $\delta_0 \rightarrow 0$ as $k \rightarrow 0$.

Suppose now that the potential, which we assume for the moment to be attractive, is multiplied by γ and we increase the coupling strength. The phase shift will then increase. In the low energy region, ka <<1, it is approximated by

$$\delta_0 \simeq ka \left(\frac{\tan \alpha a}{\alpha a} - 1 \right) \tag{80}$$

When αa lies just below the value $\pi/2$, the function in the parenthesis is large and positive until αa goes through $\pi/2$. Then the approximation (80) breaks down; the phase shift quickly turns

over and then decreases. When $\sqrt{\left(\frac{2mV_0}{\hbar^2}\right)} \cdot a = \frac{\pi}{2}$, the phase shift

has the anomalous value $\frac{\pi}{2}$ at zero energy. When $\sqrt{\left(\frac{2mV_0}{\hbar^2}\right)}$. a is slightly above $\pi/2$, then the phase shift goes through $\pi/2$ and, as

slightly above $\pi/2$, then the phase shift goes through $\pi/2$ and, as the energy decreases, keeps on increasing to π . Equation (80) must then be replaced by

$$\delta_0 \simeq \pi - ka \left(1 - \frac{\tan \alpha a}{\alpha a} \right) \qquad \dots (81)$$

Fig. 10 shows the phase-shift behaviour In the low-energy region. The solid curve represents the low-energy s-wave phase-shift for a potential not strong enough to bind. The dashed curve is for a potential that causes one loosely bound state. $\sqrt{\left(\frac{2mV_0}{\hbar^2}\right)}.a=\frac{\pi}{2}$ is precisely

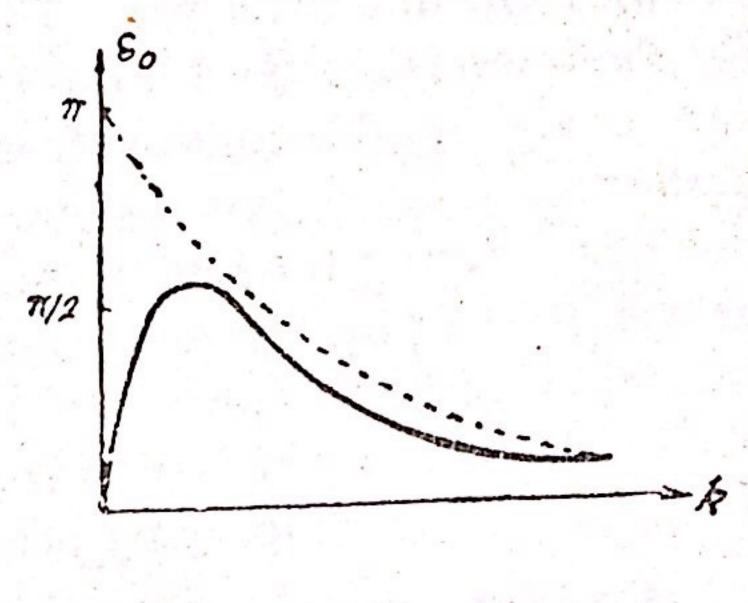


Fig. 10.

the minimum value necessary for

energy.

a bound state to exist. This is easily seen from the equation $\alpha \cot \alpha a = -|k|$

for the bound state energy $E=-\hbar^2 |k|^2/2m$. We conclude therefore that the s-wave phase shift at zero energy has the zero value is there is no bound state and the value π if there is a bound state. For the transitional values of the potential strength, the value of the s-wave phase shift at E=0 is $\pi/2$; exp. $(2i\delta_0)=-1$, and the cross-section is infinite. For the transitional potential strengths, for l=0, there is usually no bound state of zero binding

The discussion can be generalized, and one finds that every introduction of an additional bound state raises the phase shift at zero energy by an additional -. This observation says that

$$\delta_0(0) = m\pi \qquad \dots (83)$$

where m is the number of s-wave bound states; except for the "transitional" strengths, in which case

$$\delta_0(0) = (m + \frac{1}{2})\pi \tag{84}$$

These equations are known as Levinson's Theorem.

Notice that, if the potential does not bind, the phase shift does not reach $\pi/2$ and the partial cross section does not go up to its unitary limit. If the potential barely binds, the phase shift goes through $\pi/2$ in low energy region and the cross-section is maximum.

9.7. DETERMINATION OF V(r) FROM THE PHASE SHIFTS:

The theory of the preceding sections enables us to evaluate the cross section $\sigma(\theta, E)$ as a function of the angle of scattering θ and the energy E from any given potential V(r). In many situations (e.g. nucleon-nucleon and nucleon-nucleus collisions), the interac-

tion potential V(r), between the two colliding particles, is not known from first principles. Thus we try to deduce an expression for the interaction law V(r) in terms of the phase shift $\delta_l(E)$, which can easily be determined from the experimental data on the scattering cross-section $\sigma(\theta)\dagger$. Considerable literature has been published during the last twenty years on both the mathematical as well as the physical aspects of this problem. It is not possible to deal extensively with these studies in this small volume. We shall only present the basic ideas of the theory for the case where V(r) has certain simplifying properties.

From expression (45) for the Born Approximation for the phase shifts, we can write after substituting the value of $X_i^{(0)}(r)$, as

$$\sin \delta_{l} = -\frac{\lambda \pi}{2} \int_{0}^{\infty} \left[j_{l+1/2}(kr) \right]^{2} U(r) r dr$$
 ...(85)

Here we have introduced a dimensionless parameter λ as a measure of the strength of the scattering potential. Approximating $\sin \delta_l$ by δ_l , we have from (35) that

$$f(\theta) \simeq -\frac{\lambda \pi}{2k} \sum_{l} (2l+1) P_{l} (\cos \theta) \int_{0}^{\infty} [j_{l+1/2}(kr)]^{2} U(r) r dr \dots (86)$$

By means of the addition theorem for Bessel's functions

$$\frac{\sin qr}{qr} = \frac{\pi}{2kr} \sum_{l} (2l+1) \left[j_{l+1/2} (kr) \right]^2 P_l (\cos \theta).$$

where $q=2k \sin \frac{A}{2}$, and q=k-k';

we can write (86) as

$$f(\theta) = \lambda \int_0^\infty U(r) \frac{\sin q \, r}{qr} \, r^2 \, dr$$

$$\equiv -\frac{\lambda}{4\pi} \int \exp. \left[i\mathbf{q} \cdot \mathbf{r} \right] \, U(r) \, dr$$
...(37)

This is known as the first Born-Approximation for the scattering amplitude.

Choosing the direction of k+k' as the z-axis of a cylindrical coordinate system for $r(z, \rho, \phi)$, and using

^{*}Przikov, L., Ryndin, R. and Smorodinsky, J., Nuclear Physics 3,436 (1957).

$$d\mathbf{r} = dz \, d\theta \, \theta \, d\phi, \, q = 2k \sin \frac{\theta}{2}, \, z^2 = r^2 - \rho^2;$$
and
$$\int_0^{2\pi} \exp \left[i\left(2k\theta \sin \frac{\theta}{2}\right) \cos \phi\right] d\phi$$

$$= 2\pi j_0 \left(2k\theta \sin \frac{\theta}{2}\right)$$

we have
$$f(\theta) = -\frac{\lambda}{4\pi} \int_{-\infty}^{+\infty} dz \int_{0}^{\infty} \rho d\rho \ 2\pi j_0 \ U\left(\sqrt{z^2 + \rho^2}\right)$$
...(88)

On using the approximate relation ...(89) $P_t(\cos\theta) \cong j_0[(l+\frac{1}{2})\theta]$ for small θ

and setting

 $k\rho \simeq (l+\frac{1}{2}) \simeq l$ for k and l large,

and

 $2 \sin \frac{\theta}{2} \simeq \theta$ for θ small;

we can write

$$f(\theta) = -\frac{\lambda}{k^2} \int_0^{\infty} l dl \int_{r_0}^{\infty} \frac{U(r) r dr}{\sqrt{\left[r^2 - \frac{(l + \frac{1}{2})^2}{k^2}\right]}} P_l(\cos \theta) \dots (90)$$

On comparing this equation with the expression obtained from eqn. (35) as,

$$f(\theta) = \frac{1}{k} \sum_{l} (2l+1) \, \delta_{l} \, P_{l} (\cos \theta), \qquad ...(91)$$

we have the Born approximation for the phase shifts, as

$$\delta_{l} = -\frac{\lambda}{2k} \int_{0}^{\infty} \frac{U(r) \, r dr}{\sqrt{\left(r^{2} - \frac{(l + \frac{1}{2})^{2}}{k^{2}}\right)}}, \, kr_{0} = \left(l + \frac{1}{2}\right), \tag{92}$$

To solve this where we have taken l as a continuous variable. equation for V(r), we make the following substitutions:

$$\xi = \frac{1}{r^2}, \ x = \left(\frac{k}{l+\frac{1}{2}}\right)^2; \ D(x) = -\frac{2k}{\lambda} \left(\frac{l+\frac{1}{2}}{k}\right) \delta_l,$$

 $W(\xi) = \frac{1}{2} r^2 U(r),$

into it. We get the equation, known as the Abel's equation:

$$D(x) = \int_0^x \frac{W(\xi) d\xi}{\sqrt{(x - \xi)}} ...(93)$$

The solution of this equation comes out to be:

$$\lambda U(r) = \frac{4k}{\pi} \frac{d}{dr} \left[r \int_{k_{r-1/2}}^{\infty} \frac{\delta_{l} dl}{(l + \frac{1}{2})} \frac{\delta_{l} dl}{\sqrt{\left\{ \left(\frac{l + \frac{1}{2}}{k} \right)^{2} - r^{2} \right\}}} \right], \dots (94)$$

From which V(r) can be calculated if δ_i is a known function of

It is to be noted from (92) that $(k\delta_l)$ is a function of $(l+\frac{1}{2})/k$, therefore, if we write $\eta = (l+\frac{1}{2})/k$, (94) becomes

 $\lambda U(r) = \frac{4}{\pi} \frac{d}{dr} \left[r \int_{r}^{\infty} \frac{(k\delta_{l}) d\eta}{\sqrt{(\eta^{2} - r^{2})}} \right] \dots (95)$

which is independent of k. So we have calculated the potential in terms of the phase shifts, but these calculations are valid only in the special case where the potential is such that the Bornapproximation is valid. Jost and Kohn* have calculated the potential V(r) uniquely from a spectrum of δ_i (E) (i.e. the phase shifts for all energies and one given angular momentum l) for the simple case when V(r) is a repulsive potential [V(r)] is a monotonically decreasing function with $V(\infty) \rightarrow 0$, say]. Wheeler† determined V(r) from all the phase shifts δ_i (i.e., for all l) for one single energy E.

Phase Equivalent Potentials. If for some l, for which the spectrum δ_l (E) is given, there exists m discrete eigenvalues λ_l of the energy, then it is not possible to determine V(r) uniquely, but an m-fold variety of potentials, V(r), can be found that are all consistent with the δ_l (E) and the λ_l 's.

This may be understood on the following considerations: Consider the states of a given angular momentum. Let ψ_i (r) be the normalized bound state functions and ψ (k, r) the continum state functions normalized to $\sin [kr+\delta(k)]$ at large distances. If the potential U(r) is varied by an infinitesimal amount $\Delta U(r)$, the eigenvalues λ_i of the bound states and the phase shifts δ (k) will undergo the following changes:

Therefore all eigenvalues λ_i and the phase shifts $\delta(k)$ will remain unchanged if $\Delta U(r)$ is chosen to be orthogonal to the squares of all the bound states and continum eigenfunctions. It can be readily verified that the functions $\psi_i(r) \cdot \frac{d\psi_i}{dr}$ have this property. Thus an m fold variety of potentials U(r) can be constructed by forming $\Delta U(r)$ out of linear combinations of m functions

^{*}Jost, R. and Kohn, W., Phys, Rev. 87, 977 (1952); Kgl, Danska Vidensk. Mat.—fys. Nedd. 27, No. 9 (1953).

[†]Wheeler, J A, Phys, Rev, 99, 630 (1955).

 ψ_i . $\frac{d\psi_i}{dr}$, which will all have the same bound state eigenvalues λ_i and the same phase shifts $\delta(k)$. Such potentials, which give the same phase shifts are known as the Phase-equivalent Potentials.

It may be of interest to present an explicit example which forms a family of phase equivalent potentials † Let ψ (k, r) be the wave function with angular momentum zero (l=0),

$$\left(\frac{d^2}{dr^2} + k^2\right) \psi = U(r) \psi \qquad \dots (96)$$

The two independent solutions $f(\pm k, r)$ of the above equation can be chosen, which asymptotically behave as:

$$f(\pm k, r) \xrightarrow{-- \to e} \mp ikr \dots (97)$$

Now the solution ψ of (96) which satisfies the initial condition $\psi(k, r=0)=0$ can be expressed by a linear combination of $f(\pm k, r)$ as

$$\psi = \frac{1}{2i \, kr \, f(-k)} \left[f(k) \, f(-k, \, r) - f(-k) \, f(k, \, r) \right], \quad \dots (93)$$

where

$$f(k) \equiv f(k, 0); f(-k) \equiv f(-k, 0).$$
 ...(99)

The asymptotic behaviour of ψ from (98) is given as:

$$\psi \xrightarrow{r \to \infty} -\frac{1}{2ikr} \left(e^{-ikr} - \frac{f(k)}{f(-k)} e^{ikr} \right) \qquad \dots (100)$$

From (97) we get

$$f(-k, r) - f^*(k, r)$$
 and $f(-k) = f^*(k)$...(101)

So we can write (100) as:

$$\psi \xrightarrow[r \to \infty]{} -\frac{1}{2ikr} \left(e^{-ikr} - \frac{f(k)}{f^*(k)} e^{ikr} \right) \qquad \dots (102)$$

Putting $A_l = (2l+1)i^l e^{i\delta l}$ into (28) we can write the asymptotic behaviour as:

$$\psi \xrightarrow[r \to \infty]{} \Sigma \frac{1}{2kr} (2l+1) i^{l+1} \left\{ \exp \left[-i \left(kr - \frac{l\pi}{2} \right) \right] \right\}$$

exp.
$$[2i \delta_{i}(k)] \exp \left[i\left(kr-\frac{l\pi}{2}\right)\right] P_{i}(\cos \theta)$$

For zero value of the angular momentum (l=0) we have

$$\psi \xrightarrow[r \to \infty]{} -\frac{1}{2ikr} \left(e^{-ikr} - e^{2i\delta_0(k)} \cdot e^{ikr}\right) \qquad \dots (103)$$

[†]Bargmann, V., Phys Rev. 75, 30. (1949); Rev. Mod. Phys. 21, 488 (1949) (Examples of "equivalent potentials").

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Comparing (102) with (103) we see that:

$$e^{2i\delta_0(k)} = \frac{f(k)}{f''(k)}$$
 ...(104)

For the potential,

$$U(r) = \frac{\rho\sigma\{4\rho\sigma + (\rho-\sigma)^2\cosh\left[(\rho+\sigma)r - 2\theta\right] - (\rho+\sigma)^2\cosh\left(\rho-\sigma\right)r\}}{\left[\sigma\sinh\left(\rho r - \theta\right) - \rho\sinh\left(\sigma r - \theta\right)\right]^2},$$

equation (96) can be solved analytically. The solution is given

$$f(k, r) = \frac{e^{-ikr}}{\left[2k - i\left(\theta - \sigma\right)\right]\left[2k - i\left(\rho + \sigma\right)\right]} \times \left[4k^2 + \rho^2 + \sigma^2 - \frac{4ikw'}{w} - \frac{2w'}{w}\right],$$

where

 $w(r) = (\sigma e^{\rho r} - \rho e^{\sigma r}) + e^{2\theta} (\rho e^{-\sigma} - \sigma e^{-\rho r}), \theta > 0, \rho > \sigma > 0.$ and the phase shift is readily calculated as

$$\delta_0(k) = \tan^{-1} \frac{(\rho - \sigma)}{2k} + \tan^{-1} \frac{(\rho + \sigma)}{2k}$$
 ...(105)

 $\delta_0(k)$ does not depend on θ , therefore U(r) forms a family of phase-equivalent potentials for various values of θ .

9.8. SCATTERING BY COMPLEX POTENTIALS:

In many scattering problems (e.g. scattering of an electron by an atom and that of a nucleon by a nucleus), an exact treatment of the interaction between the incident particle and all the particles in the target is very complicated and difficult one. It is, therefore, desirable to devise reasonable approximations which are valid for such cases. One such approximation, known as the "optical model" has been proposed and extensively used for the collision between a nucleon and a nucleus. The basic ideas of this "optical model" are as follows:

Consider a high enery particle A incident on a composite particle P. The particle A will be scattered either elastically or inelastically. Instead of treating the interaction of A with the individual particles in P, we seek an "effective" potential V(r) between A and the whole system P, such that the scattering by V(r) can describe the observed scattering. If there is only elastic scattering, the theory is then exactly the same as treated in section 9.4.

If there is inelastic scattering, i e., the particle A is scattered after exciting P to some state, we seek an effective complex potential,

$$V(r) = V_R - iV_I,$$
 ...(106)

whose imaginary part V_I will represent the inelastic behaviour. In constructing such a potential, the choice of the strength and the shape of both the real and imaginary parts is at out disposal.

Conservation of Probability, The Schroedinger eqn. is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(\mathbf{r}, t) = i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} \qquad ...(107)$$

Thaking its complex conjugate we get:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V^*(r)\right)\psi^*(\mathbf{r},t) = -i\hbar\frac{\partial\psi^*(\mathbf{r},t)}{\partial t} \qquad \dots (108)$$

Multipying (107) by ψ^* (r, t) from left side and (108) from right by ψ (r, t) and subtracting we obtain:

$$-\frac{\hbar^2}{2m}\left[\psi^*\left(\mathbf{r},\,t\right)\,\nabla^2\psi\left(\mathbf{r},\,t\right)-\nabla^2\psi^*(\mathbf{r},\,t)\,\psi\left(\mathbf{r},\,t\right)\right]+\psi^*\left(\mathbf{r},\,t\right)$$

$$\times V(r) \psi (\mathbf{r}, t) - V^* (r) \psi^* (\mathbf{r}, t) \psi (\mathbf{r}, t) = i \hbar \left(\psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \psi \right) \dots (109)$$

Now,

$$\psi^* V \quad \psi - V^* \psi^* \psi = \psi^* \left(V_R - i \ V_I \right) \psi - \left(V_R + i V_I \right) \psi^* \psi$$

$$= 2i V_I \psi^* \psi = 2i V_I \rho \left(\mathbf{r}, t \right)$$

$$\psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \psi = \frac{\partial \left(\psi^* \psi \right)}{\partial t} = \frac{\partial \rho \left(\mathbf{r}, t \right)}{\partial t}$$

and

Hence we can write (109) as:

$$-\frac{i\hbar^{2}}{2im}\nabla\left[\psi^{*}\nabla\psi-(\nabla\psi^{*})\psi\right]-2iV_{I}\rho\left(\mathbf{r},t\right)=i\hbar\frac{\delta\rho\left(\mathbf{r},t\right)}{\delta t}$$

$$\frac{\partial\rho\left(\mathbf{r},t\right)}{\partial t}+\nabla\cdot\mathbf{S}\left(\mathbf{r},t\right)=-\frac{2V_{I}}{\hbar}\rho\left(\mathbf{r},t\right)\qquad...(110)$$

or

where the current $\overrightarrow{S}(r, t)$ is given by

$$\mathbf{S}(\mathbf{r},t) = \frac{\hbar}{2im} \left[\psi^* \nabla \psi - (\nabla \psi^*) \psi \right]$$

This is the equation of continuity for a complex potential. Since the right side in equation (110) is nonvanishing, the probability is not conserved here. As $\rho(\mathbf{r}, t)$ is positive, the r.h.s. of (110) acts as a source of probability if V_I is negative and as a sink if V_I is positive.

Absorption Scattering Cross-Section. For scattering problems, $\psi(\mathbf{r}, t)$ should be a stationary state, and hence $\rho(\mathbf{r}, t)$ will be independent of time and its derivative w.r.t. time will, therefore, vanish. Hence we can write from (110) that

$$\nabla . \mathbf{S} (\mathbf{r}, t) = -\frac{2V_I}{\hbar} \rho (\mathbf{r}, t).$$
 ...(111)

Integrating if over the entire space, we get:

$$-\int \nabla \cdot \mathbf{S} \cdot (\mathbf{r}, t) \left(d^3 r - \frac{2}{\hbar} \int V_I \rho \, d^3 r = 0 \right)$$

$$-\int_A \mathbf{S}_n \cdot d\mathbf{A} - \frac{2}{\hbar} \int_V V_I \rho \, d^3 r = 0 \qquad \dots (112)$$

For large volumes, first term on the left hand side of the above equation gives the total inward flux of particles entering the equations continued outside vanishing of it implies that the particles scattered outward are supplied by the incident planewave. Here it is the flux of particles removed from the incident plus elastically scattered wave by the complex potential, provided that ψ is normalized to a plane wave eikz of unit amplitude at infinity. It may, therefore, be set equal to $v \sigma_{ab}$, where vis the relative velocity and σ_{abs} is the total absorption crosssection. Hence we have the relation:

$$v\sigma_{abs} = \frac{2}{\hbar} \int_{V} V_{1} |\psi|^{2} d^{3}r = -\int_{A} S_{n}. dA$$

$$\sigma_{abs} = \frac{2}{\hbar v} \int_{V} V_{1} |\psi|^{2} d^{3}r = -\frac{1}{v} \int_{A} S_{n}. dA \dots (113)$$

or

Complex phase Shifts. When the potential is sherically symmetric and falls off faster than 1/r, the method of partial waves can be applied, whether the potential is real or complex. For complex potentials, the phase shifts δ_l are also complex,

$$\delta_i = \sigma_i + i\beta_i \qquad \dots (114)$$

where α_l and β_l are real.

For elastic scattering, the total scattering cross section is given by the expression (37),

$$(\sigma_{et})_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

or putting $C_i = \exp(2i \delta_i)$ we can also write,

$$(\sigma_{cl})_{tot} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |1-C_l|^2 \qquad \dots (115)$$

Now we express the total absorption scattering cross-section in terms of the phase-shifts δ_i . Choosing the surface A as the surface of a sphere of radius r, we can write from eqn. (113),

$$\sigma_{obs} = -\frac{1}{v} \lim_{r \to \infty} r^2 \int S(\mathbf{r}) \frac{d\mathbf{A}}{r^2}$$

$$= -\frac{1}{v} \lim_{r \to \infty} r^2 \int_0^{2\pi} \int_0^{\pi} S(\mathbf{r}) \sin \theta \ d\theta \ d\phi \left\{ \because \frac{d\mathbf{A}}{r^2} = d\Omega \right\}$$

$$= -\frac{1}{v} \lim_{r \to \infty} 2\pi r^2 \int_0^{\pi} S(\mathbf{r}) \sin \theta \ d\theta \quad ...(116)$$

Now the flux S(r) is given by

$$S(\mathbf{r}) = \frac{\hbar}{2im} \left(\psi^*(\mathbf{r}) \frac{\partial \psi(\mathbf{r})}{\partial r} - \frac{\partial \psi^*(\mathbf{r})}{\partial r} \psi(\mathbf{r}) \right)$$

$$\therefore \sigma_{abs} = -\frac{\hbar}{2} \frac{2\pi}{imv} \lim_{r \to \infty} r^2 \int_0^{\pi} \left(\psi^* \frac{\partial \psi}{\partial r} - \frac{\partial \psi^*}{\partial r} \psi \right) \sin \theta \, d\theta \qquad \dots (117)$$

Since $r\to\infty$ in (117), we can take the radial function $\psi(\mathbf{r})$ at asymptotic distances only. We have the asymptotic form of $\psi(\mathbf{r})$ as

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \frac{\chi_{l}(\mathbf{r})}{r} P_{l} (\cos \theta)$$
with $\chi_{l}(\mathbf{r}) \xrightarrow{r \to \infty} \frac{A_{l}}{k} \sin \left(kr - \frac{l\pi}{2} + \delta_{l} \right)$

$$(118)$$

Since δ_i is complex, therefore, $\chi_i(r)$ will also be complex, and hence

$$\psi^*(\mathbf{r}) = \sum_{l=0}^{\infty} \frac{\chi_l^*(\mathbf{r})}{r} P_l(\cos \theta) \qquad \dots (119).$$

From eqns (118) and (119) we have,

and
$$\frac{\partial \psi}{\partial r} = \sum_{l=0}^{\infty} \left(\frac{1}{r} \cdot \frac{\partial \chi_{l}}{\partial r} + 0 \left(\frac{1}{r^{2}} \right) \right) P_{l} (\cos \theta)$$

$$\vdots \int_{0}^{\pi} \left(\frac{1}{r} \cdot \frac{\partial \chi_{l}}{\partial r} + 0 \left(\frac{1}{r^{2}} \right) \right) P_{l} (\cos \theta)$$

$$\vdots \int_{0}^{\pi} \left(\psi^{*} \frac{\partial \psi}{\partial r} - \frac{\partial \psi^{*}}{\partial r} \psi \right) \sin \theta \, d\theta$$

$$= \sum_{l=0}^{\chi_{l}^{*}} \times \left(\frac{1}{r} \frac{\partial \chi_{l}'}{\partial r} + 0 \left(\frac{1}{r^{2}} \right) \right) \int_{0}^{\pi} P_{l} (\cos \theta) P_{l}' (\cos \theta) \sin \theta \, d\theta$$

$$-\sum_{l,l'} \frac{\chi_{l'}}{r} \left\{ \frac{1}{r} \frac{\partial \chi_{l}^{*}}{\partial r} + 0 \left(\frac{1}{r^{2}} \right) \right\} \right\} \int_{0}^{\pi} P_{l}(\cos \theta) P_{l'}(\cos \theta) \sin \theta \, d\theta$$

$$\text{Now} \qquad \int_{0}^{\pi} P_{l}(\cos \theta) P_{l'}(\cos \theta) \sin \theta \, d\theta = \frac{2}{(2l+1)} \delta_{ll'}.$$

$$\therefore \int_{0}^{\pi} \left(\psi^{*} \frac{\partial \psi}{\partial r} - \frac{\partial \psi}{\partial r} \psi \right) \sin \theta \, d\theta = \sum_{l} \frac{2}{(2l+1)} \cdot \frac{\chi_{l}^{*}}{r}$$

$$\times \left\{ \frac{1}{r} \frac{\partial \psi_{l}}{\partial r} + 0 \left(\frac{1}{r^{2}} \right) \right\} - \sum_{l} \frac{2}{(2l+1)} \cdot \frac{\chi_{l}}{r} \left\{ \frac{1}{r} \frac{\partial \chi_{l}^{*}}{\partial r} + 0 \left(\frac{1}{r^{2}} \right) \right\}$$

$$= \sum_{l} \frac{2}{(2l+1)} \cdot \frac{1}{r^{2}} \left(\chi_{l}^{*} \frac{\partial \chi_{l}^{*}}{\partial r} - \frac{\partial \chi_{l}^{*}}{\partial r} \chi_{l} + 0 \left(\frac{1}{r} \right) \right)$$

Hence we have

$$a_{abs} = \frac{-\pi \hbar}{2imv} \lim_{r \to \infty} \sum_{l} \frac{2}{(2l+1)} \cdot \left[\chi^* \frac{\partial \psi_l}{\partial r} - \frac{\partial \chi_l^*}{\partial r} \chi_l + 0 \right]$$

The last term on the right hand side is of the order 1/r and vanishes as are $r\to\infty$.

$$\sigma_{abs} = \frac{-2\pi \hat{\mathbf{n}}}{imv} \sum_{l} \frac{1}{(2l+1)} \left(\chi_{l}^{*} \frac{\partial \chi_{l}}{\partial r} - \frac{\partial \chi_{l}^{*}}{\partial r} \chi_{l} \right) \Big]_{r=\infty}$$

$$= \frac{2\pi i \hat{\mathbf{n}}}{\hbar k} \sum_{l} \frac{1}{(2l+1)} \left(\chi_{l}^{*} \frac{\partial \chi_{l}}{\partial r} - \frac{\partial \chi_{l}^{*}}{\partial r} \chi_{l} \right) \Big]_{r=\infty}$$

$$\{ :: mv = p = \hbar k \}$$

From eqn. (118),

$$\chi_{t}^{*} \frac{\partial \chi_{t}}{\partial r} - \frac{\partial \chi_{t}^{*}}{\partial r} \chi_{t} \xrightarrow{r \to \infty} \frac{|A_{t}|^{2}}{k} \left[\sin \left(kr - \frac{l\pi}{2} + \delta_{t}^{*} \right) \right].$$

$$\times \cos \left(kr - \frac{l\pi}{2} + \delta_{t} \right) - \cos \left(kr - \frac{l\pi}{2} + \delta_{t}^{*} \right) \sin \left(kr - \frac{l\pi}{2} + \delta_{t} \right) \left[= \frac{|A_{t}|^{2}}{k} \sin \left(-2i\beta_{t} \right) \right].$$

$$= \frac{|A_{t}|^{2}}{k} \sin \left(\delta_{t}^{*} - \delta_{t} \right) = \frac{|A_{t}|^{2}}{k} \sin \left(-2i\beta_{t} \right)$$

$$= \frac{(2l+1)^{2} e^{-2\beta t}}{k} \sin \left(-2i\beta_{t} \right) \left\{ \therefore A_{t} = (2l+1)i^{t} e^{i\omega t} \right\}.$$
or $\chi_{t}^{*} \frac{\partial \chi_{t}}{\partial r} - \frac{\partial \chi_{t}^{*}}{\partial r} \chi_{t} = \frac{(2l+1)^{2}}{k} \cdot \exp \left[-2\beta_{t} \right] \times \exp \left[-2\beta_{t} \right] \times \exp \left[-2\beta_{t} \right] = \frac{(2l+1)^{2}}{2ik} \left[1 - \exp \left(-4\beta_{t} \right) \right].$

Using it we can write

$$\sigma_{abs} = \frac{2\pi i}{k} \cdot \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)[1-\exp(-4\beta_l)]$$

$$= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)[1-\exp(-4\beta_l)]$$

$$= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)(1-|C_l|^2) \qquad \dots (121)$$

Total scattering cross-section, which is the sum of the elastic and the absorption cross-sections, is now given by

$$\sigma_{tot} = (\sigma_{el})_{tol} + \sigma_{abs}$$

$$= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left\{ | 1 - C_l|^2 + 1 - | C_l|^2 \right\}$$

$$= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left\{ 1 - C_l - C_l^* + | C_l|^2 + 1 - | C_l|^2 \right\}$$

$$= \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left[1 - \frac{C_l + C_l^*}{2} \right]$$
or
$$\sigma_{tot} = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)(1 - R_e, C_l) \qquad \dots (122)$$

Asymptotic Relations. Asymptotic behaviour of the scattering wave-function for a real potential is given by equation (11). Now we write it for a complex potential in a little more convenient form by taking A=1, the direction of the incident plane wave along the direction of k, and writing $f(k_r, k)$ in place of $f(\theta)$, where scattering is taking place from k to k_r . We have,

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow{r \to \infty} \exp \left[i\mathbf{k} \cdot \mathbf{r}\right] + \frac{f(\mathbf{k}_r, \mathbf{k})}{r} \exp \left[i\mathbf{k} \cdot \mathbf{r}\right] \dots (123)$$

or

For the initial direction - k' we have

$$\psi_{-\mathbf{k'}} \stackrel{(\mathbf{r})}{} \xrightarrow{r-\infty} \exp \left[-i\mathbf{k'} \cdot \mathbf{r}\right] + \underbrace{f(\mathbf{k_r, -k'})}_{r} \exp \left[i\mathbf{kr}\right]$$

From these asymptotic relation we shall derive two very important relations; viz., (i) the reciprocity theorem and (ii) the generalized optical theorem.

Taking the magnitudes of -k' and k the same, both will satisfy the Schroedinger equation with the same value of the energy E.

$$\begin{bmatrix}
-\frac{\hbar^2}{2m}\nabla^2 + V(r) \\
-\frac{\hbar^2}{2m}\nabla^2 + V(r)
\end{bmatrix} \psi_{\mathbf{k}}(\mathbf{r}) = E\psi_{\mathbf{k}}(\mathbf{r}) \qquad \dots (125a)$$

$$\begin{bmatrix}
-\frac{\hbar^2}{2m}\nabla^2 + V(r) \\
-\frac{\hbar^2}{2m}\nabla^2 + V(r)
\end{bmatrix} \psi_{-\mathbf{k}'}(\mathbf{r}) = E\psi_{-\mathbf{k}'}(\mathbf{r}) \qquad \dots (125b)$$

Multiplying (125 a) by $\psi_{-\mathbf{k}'}(\mathbf{r})$ and (125 b) by $\psi_{\mathbf{k}}(\mathbf{r})$ and subtracting, we get,

$$\frac{-\hbar^{2}}{2m} \left[\psi_{-\mathbf{k}'}(\mathbf{r}) \nabla^{2} \psi_{\mathbf{k}}(\mathbf{r}) - \psi_{\mathbf{k}}(\mathbf{r}) \nabla^{2} \psi_{-\mathbf{k}'}(\mathbf{r}) \right] = 0$$

$$\psi_{-\mathbf{k}'}(\mathbf{r}) \nabla^{2} \psi_{\mathbf{k}}(\mathbf{r}) - \psi_{\mathbf{k}}(\mathbf{r}) \nabla^{2} \psi_{-\mathbf{k}'}(\mathbf{r}) = 0$$

Integrating it over a large spherical volume of radius r, we get,

$$\int_{\nu} \left(\nabla \cdot \psi_{-\mathbf{k}'} (\mathbf{r}) \nabla \psi_{\mathbf{k}} (\mathbf{r}) \psi_{-\mathbf{k}} (\mathbf{r}) \nabla \psi_{-\mathbf{k}'} (\mathbf{r}) \right) = 0$$

Using Greens theorem, we can write it as a surface integral,

$$\int_{S} \left(\psi_{-\mathbf{k}'} \nabla \psi_{\mathbf{k}} - \psi_{\mathbf{k}} \nabla \psi_{-\mathbf{k}'} \right) dS = 0$$

Taking the radius of the sphere $r\to\infty$, we can write it as:

$$\lim_{r \to \infty} r^2 \int_0^{\pi} \int_0^{2\pi} \left(\psi_{-\mathbf{k}'} \frac{\partial \psi_{\mathbf{k}}}{\partial r} - \psi_{\mathbf{k}} \frac{\partial \psi_{-\mathbf{k}'}}{\partial r} \right) \sin \theta_{\mathbf{r}} d\theta_{\mathbf{r}} d\phi_{\mathbf{r}} = 0 \qquad \dots (126)$$

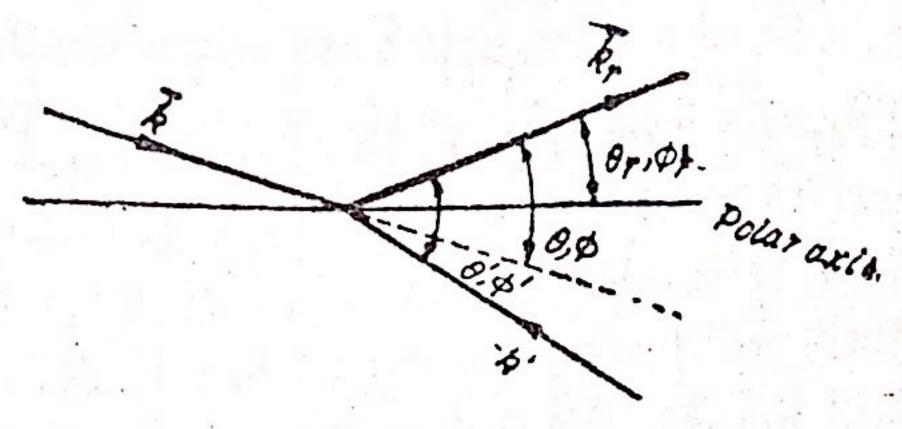


Fig. 11

where θ_r and ϕ_r are the polar angles of k_r w.r.t. some arbitrarily choosen polar axis. As we are taking $r \rightarrow \infty$ in (126), we can use the asymtotic forms (123) and (124) into it. We obtain:

Lim
$$r \ge \int_0^{2\pi} \int_0^{\pi} \left\{ ik \left(\cos \theta + \cos \theta' \right) \text{ ex. } \left\{ ikr \left(\cos \theta - \cos \theta' \right) \right\} + \frac{ik}{r} \left(1 + \cos \theta \right) f(\mathbf{k}_r, \mathbf{k}) \text{ exp. } \left\{ ikr \left(1 - \cos \theta' \right) \right\} - \frac{ik}{r} (1 - \cos \theta) f(\mathbf{k}_r, -\mathbf{k}') \text{ exp. } \left\{ ikr \left(1 + \cos \theta \right) + 0 \left(\frac{1}{r^2} \right) \right\} \times \sin \theta_r d^2 r d\phi_r = 0 \qquad \dots (127)$$

In the above integral, terms of the order $1/r^2$ vanishes in the limit $r\to\infty$, first term can be seen to vanish on integration because for every pair of angles θ , θ' , there is a caneclling pair $(\pi-\theta')$, $(\pi-\theta)$. We are thus left with,

Lim
$$r \to \infty$$
 $ikr \int_{0}^{2\pi} \int_{0}^{\pi} \left\{ (1 + \cos \theta') f(\mathbf{k}_{r}, \mathbf{k}) \exp \left\{ ikr(1 - \cos \theta') \right\} - (1 - \cos \theta) f(\mathbf{k}_{r}, -\mathbf{k}') \exp \left\{ ikr (1 + \cos \theta) \right\} \right\} \sin \theta_{r} d\theta_{r} dt_{r} = 0$

In the first terms on the left hand side of this eqn. we choose the direction of k, as the arbitrary polar axis and thus replace the variables of integration $\rho_{\mathbf{r}}$, $\rho_{\mathbf{r}}$ by $\theta_{\mathbf{r}}$, $\rho_{\mathbf{r}}$. Then, with $\mu = \cos \theta_{\mathbf{r}}$, we consider the integral,

$$I_{1}=ikr\int_{0}^{2\pi}\int_{0}^{\pi}(1+\cos\theta')f(\mathbf{k_{r}},\mathbf{k})\exp.\{ikr(1-\cos\theta')\}\sin\theta_{r}d_{r}d\phi.$$

$$=ikr\int_{0}^{2\pi}\int_{-1}^{+1}(1+\mu)f(\mathbf{k_{r}},\mathbf{k})\exp.\{ikr(1-\mu)\}d\mu\,d\phi'$$

$$=r\int_{0}^{2\pi}\int_{-1}^{+1}F_{1}(\mu,\phi')\exp.\{ikr(1-\mu)\}d\mu d\phi'\}$$
With $F_{1}(\mu,\phi')=ik(1+\mu)f(\mathbf{k_{r}},\mathbf{k})$
Calculating the μ -integral in it by parts,

$$I_{1}=r\int_{0}^{2\pi}d\phi' \left\{ |F_{1}(\mu,\phi')| \cdot \frac{i}{kr} e^{ikr(1-\mu)} \Big|_{-1}^{+1} - \frac{i}{kr} \int_{-1}^{1} \frac{\partial F_{1}}{\partial \mu} e^{ikr(1-\mu)} \right\} d\mu$$

It is apparant that further partial integration leads to successively higher powers of r in the denominator and hence the terms except the first term in the above vanishes in the limit $r \to \infty$. We thus find that

$$\lim_{r\to\infty} I_1 = \frac{i}{k} \int_0^{2\pi} d\phi' \left\{ F_1(1, \phi') - F_1(-1, \phi') e^{2ikr} \right\} \dots (129)$$

or

With the above form of $F_1(\mu, \phi')$, we see that $F_1(-1, \phi')$ vanishes.

Lim
$$r \to \infty$$
 $I_1 = \frac{i}{k} \int_0^{2\pi} F_1(1, \phi') d\phi'$
...(130)

Similarly for the second term of the equation, we have

Lim
$$r \to \infty I_2 = \lim_{r \to \infty} -ikr \int_0^{2\pi} \int_0^{\pi} (1 - \cos \theta) f(\mathbf{k}_r, -\mathbf{k}')$$

 $\times e^{ikr} (1 + \cos \theta) \sin \theta_r d\theta_r d\phi_r$

$$= -\frac{i}{k} \int_0^{2\pi} F_2(-1, \phi) d\phi$$

$$= -\frac{i}{k} \int_0^{2\pi} F_2(-1, \phi) d\phi \qquad \dots (131)$$

where $F_2(\mu, \phi) = ik(1-\mu) f(\mathbf{k_r}, -\mathbf{k'})$ and here we chose the polar axis along k. Hence we can write:

$$\int_{0}^{2\pi} F_{1} \left\{ \cos \left(\theta' = 0 \right), \, \phi' \right\} \, d\phi' - \int_{0}^{2\pi} F_{2} \left\{ \cos \left(\theta = \pi \right), \, \phi \right\} \, d\phi = 0$$

(i) Reciprocity Theorem. $\theta'=0$ on the left hand side of (132), corresponds to k, being along k' (fig. 11) and hence we can put k' for k_r in the scattering amplitude $f(k_r, k)$.

Further, the integrand is independent of ϕ' and hence the integral w.r.t. it introduces only a multiplication factor of 2π . Similarly $\theta = \pi$ on the last hand side corresponds to replacing k_r by -k in $f(k_r, -k')$ and the integration w.r.t. ϕ gives a factor of 2π . Hence we have from (132) that

$$2\pi F_{1} (\cos (\theta'=0), \phi') = 2\pi F_{2} (\cos (\theta=\pi), \phi)$$

$$ik (1+1) f(k', k) = ik (1+1) f(-k, -k')$$

$$\Rightarrow f(k', k) = f(-k, -k')$$
is known and (133)

This is known as the reciprocity theorem, which states that ...(133) the amplitude for scattering from k to k' is equal to that for the scattering from the reversed final direction -k' to the reversed initial direction -k. It is important to note that this theorem is valid for real as well as complex potential.

If the potential $V(\mathbf{r})$ is symmetric i.e., $V(\mathbf{r}) = V(-\mathbf{r})$, then all the vectors in the scattering problem may be inverted without altering the physical contents and hence we have,

$$f(-k, -k') = f(k, k')$$
 ...(134)

From (133) and (134) we obtain a slightly specialized reciprocity theorem:

$$f(k', k) = f(k, k')$$
 ...(135)

(ii) Generalized Optical Theorem. Taking the complex conjugate of the Schroedinger equation $\psi_{\mathbf{k}}$, we get

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{(r)}^* \right] \psi_{\mathbf{k}'}^*(\mathbf{r}) = E \psi_{\mathbf{k}'}^*(\mathbf{r}) \qquad ...(136)$$

Multiplying the Schroedinger equation for $\psi_{\mathbf{k}}(\mathbf{r})$ by $\psi_{\mathbf{k}}^*$, (r) and (136) by $\psi_{\mathbf{k}}(\mathbf{r})$ and subtracting, we have:

$$\frac{-\hbar^{2}}{2m} \left[\begin{array}{ccccc} \psi_{\mathbf{k}'}^{*} & \nabla^{2} \psi_{\mathbf{k}} - \psi_{\mathbf{k}} & \nabla^{2} \psi_{\mathbf{k}'}^{*} \end{array} \right] - 2i V_{I} \psi_{\mathbf{k}'}^{*}, \psi_{\mathbf{k}} = 0$$

$$\{ : V = V_{R} - iV_{I} \}$$

Integrating this equation over the entire space,

$$\left[\left(\psi_{\mathbf{k}}^*, \nabla^2 \psi_{\mathbf{k}} - \psi_{\mathbf{k}} \nabla^2 \psi_{\mathbf{k}'}^* \right) d^3r + \frac{4mi}{\hbar^2} \right] V_I \psi_{\mathbf{k}'}^* \psi_{\mathbf{k}} d^3r = 0$$

Using Greens theorem in the first integral on the left hand side, we obtain

$$\left(\left(\psi_{\mathbf{k}'}^* \nabla \psi_{\mathbf{k}} - \psi_{\mathbf{k}} \nabla \psi_{\mathbf{k}'}^* \right)_n dS + \frac{4mi}{\hbar^2} \int V_1 \psi_{\mathbf{k}'}^* \psi_{\mathbf{k}} d^3 r = 0...(137) \right)$$

To evaluate the first integral in the above, we take the surface as the surface of a sphere of radius r and take the limit $r \rightarrow \infty$. Hence we have the first term as:

$$\lim_{r \to \infty} r^2 \int \left(\psi_{\mathbf{k}'}^* \frac{\partial \psi_{\mathbf{k}}}{\partial r} - \psi_{\mathbf{k}} \frac{\partial \psi_{\mathbf{k}'}^*}{\partial r} \right) \sin \theta_r \, d\theta_r \, d\phi_r \qquad \dots (138)$$

Using the Asymptotic form (123), it can be written as:

Lim
$$r^{2} \int_{0}^{2\pi} \int_{0}^{\pi} d\phi_{r} \sin \theta_{r} d^{3}r$$

 $\times \left[ik \left(\cos \theta + \cos \theta' \right) \exp \left(ikr \left(\cos \theta - \cos \theta' \right) \right) + \left(\frac{ik}{r} (1 + \cos \theta') - \frac{1}{r^{2}} \right) f(\mathbf{k}_{r}, \mathbf{k}) \exp \left(ikr (1 - \cos \theta') \right) + \left(\frac{ik}{r} (1 + \cos \theta) + \frac{1}{r^{2}} \right) f^{*}(\mathbf{k}_{r}, \mathbf{k}') \exp \left(-ikr (1 - \cos \theta) \right) + \left(\frac{2ik}{r^{2}} f^{*}(\mathbf{k}_{r}, \mathbf{k}') f(\mathbf{k}_{r}, \mathbf{k}) \right) + \frac{4mi}{\hbar^{2}} \int V_{I} \psi_{\mathbf{k}'}^{*} \psi_{\mathbf{k}} d^{3}r = 0 \dots (139)$

As in eqn. (127), the first term in the first integral on the left hand side gives zero and the terms containing $1/r^2$ can also be neglected. The two remaining exponential terms are exactly I_1 and I_2 . The first term will have $\cos \theta' = 1$ or $k_r = k'$ axid the second term has $\cos \theta = 1$ or $k_r = k$. Thus we get:

人

414
$$-4\pi f(\mathbf{k}', \mathbf{k}) + 4\pi f^{*}(\mathbf{k}, \mathbf{k}')$$

$$+2ik \int_{0}^{2\pi} \int_{0}^{\pi} f^{*}(\mathbf{k}_{r}, \mathbf{k}') f(\mathbf{k}_{r}, \mathbf{k}) \sin \theta_{r} d\theta_{r} d\phi_{r}$$

$$+\frac{4mi}{\hbar^{2}} \int V_{I} \psi_{\mathbf{k}'}^{*} \psi_{\mathbf{k}} d^{3}r = 0 \qquad ...(140)$$

We now consider the following two cases

(I) V(r) is real. Here $V_1=0$ and hence (140) gives:

(I)
$$V(\mathbf{r})$$
 is read.

(I) $f(\mathbf{k}_r, \mathbf{k}') f(\mathbf{k}_r, \mathbf{k}) \sin \theta_r d\theta_r d\phi_r = \frac{-2\pi i}{k} [f(\mathbf{k}', \mathbf{k}) - f^*(\mathbf{k}, \mathbf{k}')]$
...(141)

If the potential is symmetric, then from the Reciprocity theorem we have the eqn. (141) as:

$$\int_{0}^{2\pi} \int_{0}^{\pi} f^{*}(\mathbf{k}', \mathbf{k}_{r}) f(\mathbf{k}_{r}, \mathbf{k}) \sin \theta_{r} d\theta_{r} d\phi_{r} = \frac{4\pi}{\mathbf{k}} I_{m} f(\mathbf{k}', \mathbf{k}) ...(142)$$

This relation is known as the generalized optical theorem.

(II) k'=k. In this case the volume integral in (140) has a simple physical interpretation. Since,

$$\int V_I \psi_{\mathbf{k}'}^*, \ \psi_{\mathbf{k}} d^3r = \frac{1}{2}\hbar v \ \sigma_{abs.},$$

we can write (140) as:

$$\int_{0}^{2\pi} \int_{0}^{\pi} |f(\mathbf{k}_{r}, \mathbf{k})|^{2} \sin \theta_{r} d\theta_{r} d\theta_{r} + \sigma_{abs} = \frac{4\pi}{k} I_{m}.f(\mathbf{k}, \mathbf{k})$$

First term on the left hand side is total elastic cross-section σ_{el} , so that the left hand side is equal to σ_{tot} . We thus obtain the optical theorem;

$$\sigma_{tot.} = \frac{4\pi}{k} I_m. f(\mathbf{k}, \mathbf{k}) \qquad \dots (143)$$

This theorem is applicable even if V is neither symmetric nor real.

Open and Closed Channel. The concept of channel is very useful in the treatment of complex collisions. A channel is any possible mode of scattering of the incident and the scattering particles to the final state. One of these modes is the incident particle and the scatterer themselves: it is called the entrance channel. In an elastic scattering, the two particles remain in the entrance channel. If scattering causes a change in the internal energy of the particles, we call it as the inelastic scattering. In this case, the out-going channel is different from the entrance channel. This is another example of a channel. Sometimes the incident particle exchange a certain number of its constituent

elementary particles with the scatterer in the course of the collision. This is called as a rearrangement collision. A chemical reaction is a rearrangement collision between molecules and a nuclear reaction is a rearrangement collision between atomic nuclei. There may be various channels in a rearrangement collision which are distinguished by different internal energies and different nature of the two fragments in the final state. We shall henceforth denote a channel by a particular Greek letter. With each channel we may associate a certain number of parameters and magnitudes. For simplicity, we shall always assume that the channels are made up of two particles.

Let us consider a channel α made up of two particles, A and B. The wave function ψ_{α} , describing the internal quantum state of the particles of the channel is the product of the wave functions ψ_A and ψ_B for the particles A and B, respectively. If H_A and H_B are the Hamiltonians of these particles, then we have

$$H_A \psi_A = E_A \psi_A \qquad H_B \psi_B = E_B \psi_B$$

$$\psi_\alpha = \psi_A \psi_B \qquad E_\alpha = E_A + E_B \qquad ...(144)$$

 E_{α} is the total internal energy of the particles of channel α . If V_{α} be the interaction between particles A and B, then the Hamiltonian of the system is given by

$$H = H_{\alpha} + V_{\alpha} \qquad \dots (145)$$

with

$$H_{\alpha} = H_A + H_B + \frac{P_{\alpha}^2}{2M_{\alpha}},$$
 ...(146)

where, P_{α} is the relative momentum of the particles in the initial state, and M_{α} is their reduced mass,

$$M_{\alpha} = \frac{M_A M_B}{M_A + M_B}.$$

Thus the total energy of the channel a is given by;

$$E = E_{\alpha} + \hbar^2 k_{\alpha}^2 / 2M_{\alpha} \qquad ...(147)$$

If the outgoing channel β is made up of the particles C and D and $\hbar k_{\beta}$ is the relative momentum, then from the conservation of energy,

$$E = E_{\beta} + \hbar^2 k^2_{\beta} / 2M_{\beta} \qquad ...(148)$$

where E_{β} is the internal energy of the outgoing channel. For a given total energy E, it may be possible to excite some internal energy levels and still have some (positive) kinetic energy " $(E-E_{\beta})$ " of the fragments left over; other levels may not be so accessible. The channels corresponding to the former are said to

be open, and those corresponding to the latter are said to be closed. The energy at which a channel opens up is its threshold.

9.9. GREEN'S FUNCTIONS IN SCATTERING THEORY:

Let us consider the scattering of a particle by a potential $V(\mathbf{r})$ of *finite range*. The Schroedinger equation to be solved for the system is

where, $k^2 = 2mE/\hbar^2$ and $U(\mathbf{r}) = U(\mathbf{r}) \psi(\mathbf{r})$... (149)

This equation can very easily be solved by Green's function technique, if we assume the right hand side of it temporarily as a given inhomogeneity, though it contains the unknown function $\psi(\mathbf{r})$. We define the Green's function $G(\mathbf{r}, \mathbf{r}')$ as the effect at the observer's point ' \mathbf{r} ' in a cause-effect relationship, by a unit point source at the source point " \mathbf{r} ". Thus the effect at \mathbf{r} caused by a source distribution $F(\mathbf{r}')$ [strength of the source per unit volume] is the integral of $G(\mathbf{r}, \mathbf{r}') F(\mathbf{r}')$ over the whole range of \mathbf{r}' occupied by the source,

Total Effect at
$$\mathbf{r} = \int_{V'} G(\mathbf{r}, \mathbf{r}') F(\mathbf{r}') d^3\mathbf{r}'$$
 ...(150)

In equation (149), right hand side can be identified as the source function $F(\mathbf{r})$. Hence the Green's function for the solution of (149) will be the solution of an equation obtained by replacing the r.h.s. by the unit point source $\delta(\mathbf{r}-\mathbf{r}')$ at point \mathbf{r}' , i.e,

$$(\nabla^2 + k^3) G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$
 ...(151)

Thus a particular solution of (149) can be written by taking analogy from (150), as:

$$\psi(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \phi(\mathbf{r}') d^3r'$$
 ...(152)

In order to get the complete solution of (149) we should add an arbitrary solution ϕ (r) of the homogeneous equation,

 $(\nabla^2 + k^2) \phi(\mathbf{r}) = 0$...(153)

Thus the complete solution of (149) can be written as:

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + \int G(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') d^3r' \dots (154)$$

$$0 \text{ obtain } G(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') d^3r'$$

Now, to obtain $G(\mathbf{r}, \mathbf{r}')$ we have to solve equation (151). For it we write the Fourier Transforms of G and δ as:

$$G(\mathbf{r}, \mathbf{r}') = \int g(\mathbf{k}') \exp \{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\} d^3k',$$
and
$$\delta(\mathbf{r} - \mathbf{r}') = \frac{1}{(2\pi)^8} \int \exp \{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')\} d^3k'$$
...(155)

Substituting these into (151) we get:

$$\int (-k'^2 + k^2) g (k') \exp \{ik' \cdot (r - r')\} d^3k'$$

$$= \frac{1}{(2\pi)^3} \int \exp \{ik' \cdot (r - r')\} d^3k'.$$

From it we see that

$$(-k^{2}+k^{2}) g(\mathbf{k}') = \frac{1}{(2\pi)^{3}} \text{ or } g(\mathbf{k}') = \frac{1}{(2\pi)^{3}} \frac{1}{k^{2}-k^{2}}.$$

Using this value of g(k') we can write,

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi)^3} \int \frac{\exp \left\{ik' \cdot (\mathbf{r} - \mathbf{r}')\right\}}{k^2 - k'^2} d^3k'$$

$$= \frac{1}{(2\pi)^3} \int \frac{\exp \left\{ik' \mid \mathbf{r} - \mathbf{r}' \mid \cos \theta_{k'}\right\}}{k^2 - k'^2} k'^2 dk' \sin \theta_{k'} d\theta_{k'} d\phi_{k'}$$

$$= \frac{2}{4\pi^2 \mid \mathbf{r} - \mathbf{r}' \mid i} \int_0^\infty \frac{\sin \left(k' \mid \mathbf{r} - \mathbf{r}' \mid\right)}{k^2 - k'^2} k' dk'$$

$$= \frac{1}{4\pi^2 \mid \mathbf{r} - \mathbf{r}' \mid i} \int_{-\infty}^{+\infty} \frac{\exp \left\{ik' \mid \mathbf{r} - \mathbf{r}' \mid\right\}}{k^2 - k'^2} dk' \dots (156)$$

Integrand of the integral in (156) has got two simple poles on the real axis at $k'=\pm k$. To evaluate (156) we can choose the contour in the upper half plane or in the lower half plane as shown in fig. (12). The path of the integration leads along the real axis from $-\infty$ to $+\infty$. If we close the contour in the upper half plane, it encloses the singularity in the right half-plane in accordance with the Jordan's lemma. If we close the contour in the

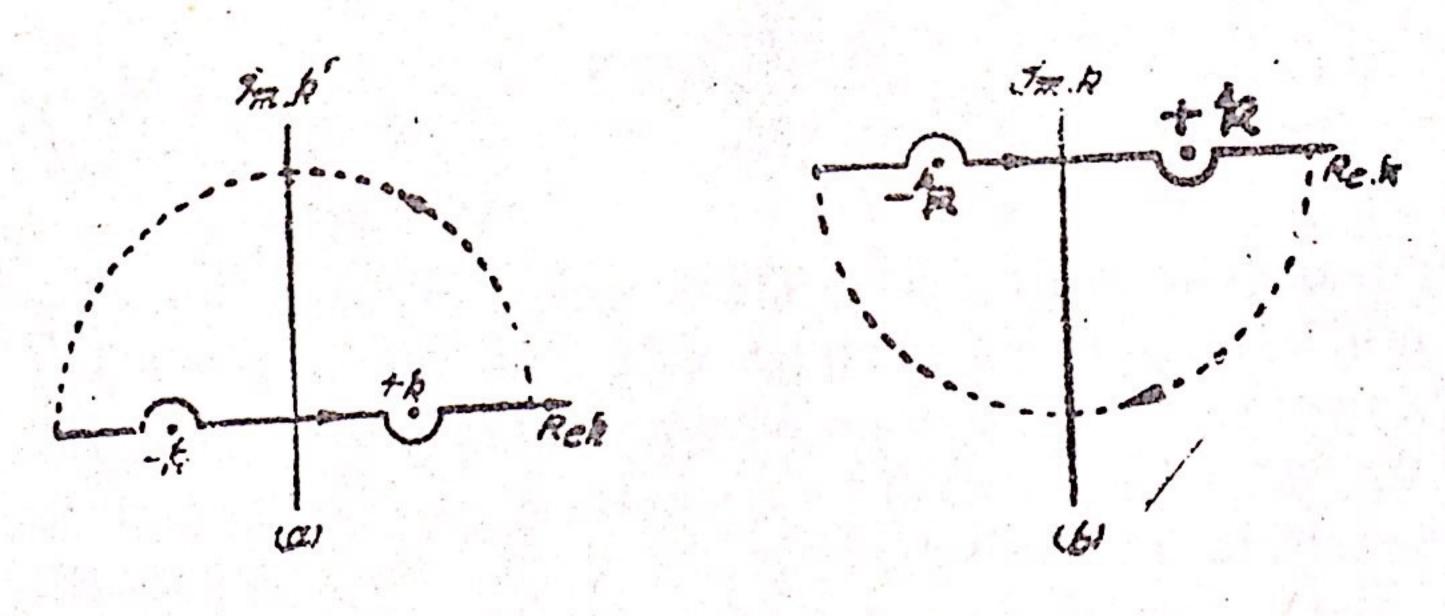


Fig. 12.

lower half-plane, it encloses the singularity in the left half plane. Thus we get two types of Green's function corresponding to the two ways of enclosing the contour. If we consider the coutour of fig. 12 (a), we get the following Green's function,

$$G^{(+)}(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi^{2} |\mathbf{r} - \mathbf{r}'| i} \cdot 2\pi i \times (\text{residue of integrand at } k' = k)$$

$$= \frac{1}{4\pi^{2} |\mathbf{r} - \mathbf{r}'| i} \cdot 2\pi i \cdot \lim_{k' \to k} \frac{\exp \cdot \{ik' |\mathbf{r} - \mathbf{r}'|\} \cdot k' (k' - k)}{(k - k')(k + k')}$$

$$= \frac{-1}{4\pi^{2} |\mathbf{r} - \mathbf{r}'| \cdot 2\pi \cdot \frac{\exp \cdot \{ik |\mathbf{r} - \mathbf{r}'|\}}{2}$$

$$= \frac{-1}{4\pi} \cdot \frac{\exp \cdot \{ik |\mathbf{r} - \mathbf{r}'|\}}{|\mathbf{r} - \mathbf{r}'|} \dots (157-a)$$

Similarly taking the contour of fig. 12 (b) we get:

$$G^{(-)}(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi^2 |\mathbf{r} - \mathbf{r}'| i} - 2\pi i \times (\text{residue of integrand at } k' = -k)$$

$$= \frac{-1}{4\pi} \cdot \frac{\exp \left\{-ik | \mathbf{r} - \mathbf{r}'|\right\}}{|\mathbf{r} - \mathbf{r}'|} \dots (157-b)$$

Corresponding to (157-a and b) we get the solutions of (149)

as:

$$\psi^{(\pm)}(\mathbf{r}) = (\phi)(\mathbf{r}) - \frac{1}{4\pi} \int \frac{\exp \left\{ \pm ik \mid \mathbf{r} - \mathbf{r}' \mid \right\}}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}') \psi^{(\pm)}(\mathbf{r}') d^{3}r'$$
...(158)

To calculate the scattering cross-section, we need the asymptotic behaviour of the solutions (158). For finding it, we have

$$|\mathbf{r} - \mathbf{r}'| = (r^2 + r'^2 - 2\mathbf{r} \cdot \mathbf{r}')^{1/2}$$

$$= r \left(1 - \frac{2\mathbf{r} \cdot \mathbf{r}'}{r^2} + \frac{r'^2}{r^2}\right)^{1/2}$$

$$= r \left(1 - \frac{\mathbf{r} \cdot \mathbf{r}'}{r^2} + \frac{r'^2}{2r^2} + \dots\right) \quad \{\text{Expanding Binomially}\}$$

Now from the fact that U(r') in the integrand in (158) is non-zero only for a finite region, we can neglect the terms of order $\left(\frac{r'}{r}\right)$ and higher in the expansion for asymptotic regions $(r \to \infty)$.

$$\therefore |\mathbf{r} - \mathbf{r}'| \xrightarrow{- \to r} \left(1 - \frac{\mathbf{r} \cdot \mathbf{r}'}{r^2}\right) = r - \frac{\mathbf{r}}{r} \cdot \mathbf{r}' = r - \hat{n} \cdot \mathbf{r}' \quad ... \quad (159)$$

where, \hat{n} is a unit vector along the direction of vector \mathbf{r} .

Similarly,
$$\frac{1}{|\mathbf{r} - \mathbf{r'}|} = \frac{1}{r} \left(1 - \frac{2\mathbf{r} \cdot \mathbf{r'}}{r^2} + \frac{r'^2}{r^2} \right)^{-1/2}$$
$$= \frac{1}{r} \left(1 + \frac{\mathbf{r} \cdot \mathbf{r'}}{r^2} - \frac{r'^2}{2r^2} - \dots \right)$$

$$\Rightarrow \frac{1}{|\mathbf{r}-\mathbf{r'}|} \xrightarrow{r \to \infty} = \frac{1}{r} \qquad \dots (160)$$

Using (159) and (160) into (154), we get the asymptotic behaviour as:

$$\psi^{(\pm)}(\mathbf{r}) \xrightarrow{r \to \infty} \phi(\mathbf{r}) - \frac{1}{4\pi} \int \frac{\exp\left(\pm ik\left(r - \hat{n} \cdot \mathbf{r}'\right)\right)}{r} \times U(\mathbf{r}') \psi^{(\pm)}(\mathbf{r}') d^3r' \dots (161)$$

Since ϕ (r) is the solution of the free particle wave equation (153), $\psi^{(\pm)}$ (r) can be recognized as a plane wave plus an outgoing wave and $\psi^{(-)}$ (r) represents as a plane wave plus an incoming wave. In scattering experiments, detector is placed outside the region of the incident beam and we observe only the scattered part. We thus restrict ourselves to the solution corresponding to the outgoing wave only,

$$\psi^{(\pm)}(\mathbf{r}) = \phi(\mathbf{r}) - \frac{1}{4\pi} \cdot \frac{\exp(ikr)}{r} \int \exp(-ik\hat{n}\cdot\mathbf{r}') U(\mathbf{r}') \psi^{(\pm)}(\mathbf{r}') d^3r'$$
...(162)

This equation is exactly of the form of equation (11), with A=1; and comparing it with eqn. (11), we obtain the scattering amplitude as:

$$f(\theta) = -\frac{1}{4\pi} \int \exp \left\{-ik\hat{n} \cdot \mathbf{r}'\right\} U(\mathbf{r}') \psi^{(+)}(\mathbf{r}') d^3r' \qquad \dots (163)$$

Once $f(\theta)$ is known, the differential scattering cross-section and the total scattering cross-section can be calculated easily from eqns. (13) and (14); respectively.

9.10. BORN APPROXIMATION:

The wave function for the scattering of a particle by a potential $V(\mathbf{r})$ is given by:

$$\psi^{(+)} = \exp \{ik \cdot \mathbf{r}\} + \int G^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \psi^{(+)}(\mathbf{r}') d^3r', \dots (164)$$

where we have written the plane wave exp. $\{i\mathbf{k} \cdot \mathbf{r}\}$ for the free particle wave function $\phi(\mathbf{r})$, $U(\mathbf{r})=2m\ V(\mathbf{r})/\hbar^2$ and G^+ is the Green's function (157-a).

This is an integral equation for $\psi^{(+)}$ and can be solved by the method of successive substitutions. After first substitution we get:

$$\psi^{(+)}(\mathbf{r}) = \exp \{i\mathbf{k} \cdot \mathbf{r}\} + \int G^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \left[\exp \{i\mathbf{k} \cdot \mathbf{r}'\} + \int G^{(+)}(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'') \psi^{(+)}(\mathbf{r}'') d^3r''\right] d^3r'$$

=exp.
$$\{ik.r\}+\int G^{(+)}(\mathbf{r},\mathbf{r}')\ U(\mathbf{r}')\ \exp.\ \{ik.r'\}\ d^3r'$$

+ $\iint G^{(+)}(\mathbf{r},\mathbf{r}')\ U(\mathbf{r}')\ G^{(+)}(\mathbf{r}',\mathbf{r}'')\ U(\mathbf{r}'')\ \psi^{(+)}(\mathbf{r}'')\ d^3r'\ d^3r''.$

Going on substituting like it, after an infinite number of step, we obtain

$$\psi^{(+)}(\mathbf{r}) = \exp \{i\mathbf{k}.\mathbf{r}\} + \int G^{(+)}(\mathbf{r}, \mathbf{r}') \ U(\mathbf{r}') \exp \{i\mathbf{k}.\mathbf{r}'\} \ d^{3}r'$$

$$+ \iint G^{(+)}(\mathbf{r}, \mathbf{r}') \ U(\mathbf{r}') \ G^{(+)}(\mathbf{r}', \mathbf{r}'') \ U(\mathbf{r}'') \exp \{i\mathbf{k}.\mathbf{r}''\} \ d^{3}r' \ d^{3}r''$$

$$+ \iiint G^{(+)}(\mathbf{r}', \mathbf{r}') \ U(\mathbf{r}') \ G^{(+)}(\mathbf{r}', \mathbf{r}'') \ U(\mathbf{r}'') \ G^{(+)}(\mathbf{r}'', \mathbf{r}''') \ U(\mathbf{r}'')$$

$$\times \exp \{i\mathbf{k}\cdot\mathbf{r}'''\} \ d^{3}r'' \ d^{3}r''' \ d^{3}r''' \(165)$$

This series is known as the Born Series. To sum the infinite number of terms in this series is really very tedius. However, if the potential U(r) is weak, the series can be well approximated by a first few terms only. This is called Born Approximation. If we keep the first two terms in the series, we get the first Born approximation, first three terms give the second Born approximation, and so on. For very-very weak potentials, first Born approximation is a very good approximation.

It is usually referred to as the Born Approximation. In this approximation we get,

 $\psi^{(+)}(\mathbf{r}) = \exp[[i \mathbf{k} \cdot \mathbf{r}] + \int G^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \exp[[i \mathbf{k} \cdot \mathbf{r}']] d^3r' \dots (166)$ i.e., it is equivalent to replacing the wave-function $\psi^{(+)}(\mathbf{r}')$ under the integral on the right hand side of (164) by the plane wave exp. $(i\mathbf{k}\mathbf{r}')$. When the potential is very weak it is quite justified because the wave-function $\psi^{(+)}(\mathbf{r}')$ will deviate only slightly from the free particle plane wave exp. $[i\mathbf{k} \cdot \mathbf{r}']$.

Using (157-a) and, (159) and (160) we can write the asymptotic form of (166) as:

$$\psi^{(+)}(\mathbf{r}) \xrightarrow{r \to \infty} \exp[i\mathbf{k} \cdot \mathbf{r}] - \frac{1}{4\pi} \cdot \frac{\exp[i\mathbf{k}r]}{r} \times$$

 $\int \exp \left[-i\hat{k}n.\mathbf{r}'\right]U(\mathbf{r}')\exp \left[i\mathbf{k}.\mathbf{r}'\right]d^3r'$...(167) Comparing it with the asymptotic form,

$$\psi(\mathbf{r}) \xrightarrow{r \to \infty} \exp \left[ikz\right] + \frac{f(\theta)}{r} \exp \left[ikr\right],$$

we find that the scattering amplitude in first Born Approximation is given by:

$$f(\theta) = -\frac{1}{4\pi} \int \exp \left[-ik\hat{n} \cdot \mathbf{r}'\right] U(\mathbf{r}') \exp \left[ik \cdot \mathbf{r}'\right] d^3r'$$

$$= -\frac{1}{4\pi} \cdot \frac{2m}{\hbar^2} \int \exp \left[-ik' \cdot \mathbf{r}'\right] V(\mathbf{r}') \exp \left[ik \cdot \mathbf{r}'\right] d^3r' \dots (168)$$

Because \hat{n} is a unit vector along the direction of scattering \hat{r} hence $k\hat{n}$ is the scattered wave vector k', as |k| = |k'| = k for elastic scattering.

Now h k is the momentum of the incident particle and hk is the momentum of the scattered particle; the momentum transferred from incident particle to the scattering potential during collision is given by:

$$\hbar K = \hbar k - \hbar k'$$
 ...(169)

With these notations eqn. (168) becomes;

$$f(\theta) = -\frac{1}{4\pi} \cdot \frac{2m}{\hbar^2} \int \exp \left[i\mathbf{K} \cdot \mathbf{r'}\right] V(\mathbf{r'}) d^3r'$$
 ...(170)

If the potential is spherically symmetric, i.e., $V(\mathbf{r}') = V(r')$; we can further write it as:

$$f(\theta) = -\frac{2m}{4\pi\hbar^2} \int \exp \left[i K r' \cos \theta'\right] V(r') r'^2 dr' \sin \theta' d\theta' d\phi'$$

$$= -\frac{2m}{\hbar^2 K} \int_0^\infty r' \sin K r' V(r') dr' \qquad ... (171)$$

If V(r) is an even-function of r, we can also write it as

$$f(\theta) = -\frac{m}{\hbar^2 Ki} \int_{-\infty}^{+\infty} r' \exp(i K r') V(r') dr'$$
 ...(172)

Expressions (171) and (172) give the scattering amplitudes under Born Approximation. From it we can find the differential and the total scattering cross-sections.

Validity Criteria for Born Approximation. As discussed above, the Born approximation is a good approximation only when the incident wave is distorted negligibly by the potential. This happens when the potential is weak and the incident energy is very high. To derive a mathematical relation for the validity, we require in equation (166) that,

$$\int G^{(+)}(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \exp[i \mathbf{k} \cdot \mathbf{r}'] d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}'] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}'] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | d^3r' | \langle \langle | \exp[i \mathbf{k} \cdot \mathbf{r}] | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r' | d^3r'$$

or
$$\left| -\frac{2m}{\hbar^2} \cdot \frac{1}{4\pi} \int \frac{\exp \left[i k | \mathbf{r} - \mathbf{r}'|\right]}{|\mathbf{r} - \mathbf{r}'|} V(\mathbf{r}') \exp \left[i k \cdot \mathbf{r}'\right] d^3r' \right| \langle \langle 1 \rangle$$

It is convenient to satisfy this condition at the origin (r=0). Since the potential is strongest at the centre of the scattering, the resulting validity criterion is sufficient for all values of r. Hence we write,

 $\left| -\frac{2m}{\hbar^2} \cdot \frac{1}{4\pi} \cdot \int \frac{\exp \left[i k r'\right]}{r'} V(\mathbf{r}') \exp \left[i k \cdot \mathbf{r}\right] \right|$

 $r'^2 dr' \sin \theta' d\theta' d\phi' \langle \langle 1.$

If $V(\mathbf{r}')$ is spherically symmetric, then this expression can be written as:

writen as
$$\left| -\frac{2m}{\hbar^2} \cdot \frac{1}{4\pi} \cdot \frac{4\pi}{k} \int_0^\infty \exp\left[i k r'\right] \sin k r' V(r') dr' \right| \langle \langle 1 \rangle$$
or
$$\frac{2m}{\hbar^2 k} \left| \int_0^\infty \exp\left[i k r'\right] \sin k r' V(r') dr' \right| \langle \langle 1 \rangle \rangle ...(173)$$

This can also be written as:

$$\frac{m}{\hbar^2 k} \left| \int_0^\infty \exp(2i \, kr') - 1 \right| V(r') \, dr' \left| \langle \langle 1 \rangle \rangle \right| ... (174)$$

9.11. ELECTRON ATOM SCATTERING:

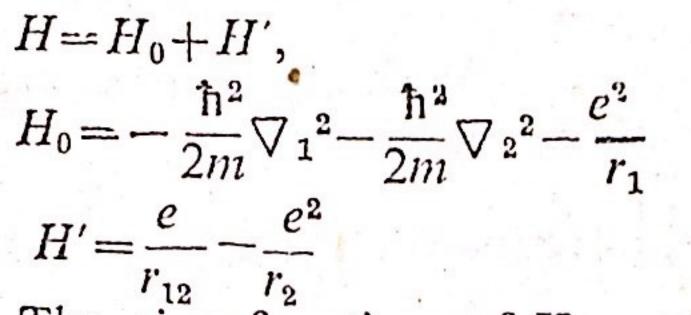
Electron atom scattering differs from the ordinary potential scattering in the following respects:

- (i) The scatterer has an infinite number of internal degrees of freedom, so that it can be excited during the scattering process, for example, an electron may be scattered by an atom which is initially in its ground state; and after the collision, the atom may be left in its ground state (elastic scattering) or in an excited state (inelastic scattering).
- (ii) The incident electron may be exchanged with an atomic electron and hence the exchang effects may occur in the collision.
- (iii) The incident electron produces an electric field which can polarize the target atom and hence the polarization effects are also involved.

If we consider the energy of the incident electron as very high, the exchange and the polarization effects are unimportant and can be ignored.

We divide the total Hamiltonian into a part H_0 that describes the internal motion of the atom together with the kinetic

energy of the relative motion of the incident electron and the scatterer atom, and a part H' which represents the interaction between the incident particle and the scatterer. For example, in the scattering of an electron (co-ordinate r_2) by a hydrogen atom (atomic-electron coordinate r_1) we have,



The eigenfunctions of H_0 are specified by two parameters:

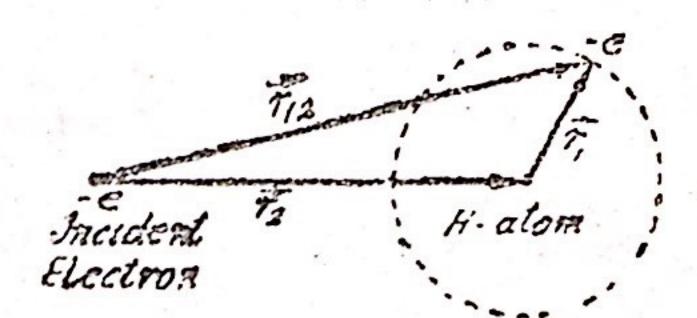


Fig. 13.

$$H_0 \phi_{\alpha a}(\mathbf{r}_1, \mathbf{r}_2) = E_{\alpha a} \phi_{\alpha a}(\mathbf{r}_1, \mathbf{r}_2)$$
 ...(1.5)

Here α -specifies the initial quantum state of the incident electron and α -specifies that of the atom. We can write,

$$\phi_{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2) = w_{\alpha}(\mathbf{r}_1) \phi_{\alpha}(\mathbf{r}_2), \qquad ...(176)$$

where $w_{\alpha}(\mathbf{r}_1)$ is the unperturbed wave-function for the atom and $\phi_{\alpha}(\mathbf{r}_2) = \exp$. ($i \mathbf{k}_{\alpha} \cdot \mathbf{r}_2$) is the free particle wave-function for the incident electron,

$$E_{\alpha a} = E_{\alpha} + \in_{\alpha} \qquad ... (177)$$

where, E_{α} is the kinetic energy of the incident free electron and \in_{α} are the unperturbed eigenvalues of the atom.

Now the wave-function, $\psi_{\alpha a}^{(+)}$, of the total Hamiltonian H can be written analogous to eqn. (164) as:

$$\psi_{\alpha a}^{(+)}(\mathbf{r}_{1}, \mathbf{r}_{2}) = \phi_{\alpha a}(\mathbf{r}_{1}, \mathbf{r}_{2}) + \frac{2m}{\hbar^{2}} \iint G_{\alpha a}^{(+)}(\mathbf{r}_{1}, \mathbf{r}_{2}; \mathbf{r}_{1}, \mathbf{r}_{2}') \times H'(\mathbf{r}_{1}', \mathbf{r}_{2}') \psi_{\alpha a}^{(+)}(\mathbf{r}_{1}', \mathbf{r}_{2}') d^{3}r'_{1} d^{3}r'_{2}', \dots (178)$$

where $G_{\alpha a}^{(+)}$ (r, r_2 ; r'_1 , r'_2)† is the Green's function for the solution (178).

†Green function $G^{(+)}_{\alpha\alpha}$ $(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r'}_1, \mathbf{r'}_2)$ is given by:

$$G_{\alpha\alpha}^{(+)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = \frac{-1}{4\pi} \left[w_b^*(\mathbf{r}'_1) w_\alpha(\mathbf{r}_1) \frac{\exp[ik_\alpha | \mathbf{r}_2 - \mathbf{r}'_2|]}{|\mathbf{r}_2 - \mathbf{r}'_2|} \right]$$

Hence we have its asymptotic behaviour as;

$$G_{2a}^{(+)} \xrightarrow[r_2 \to \infty]{} \frac{-1}{4\pi} \int w_b^* (\mathbf{r}'_1) w_a (\mathbf{r}_1) \frac{\exp [ik_a (\mathbf{r} - \hat{\mathbf{n}} \cdot \mathbf{r}'_2)]}{\mathbf{r}_2}$$

where \hat{n} is a unit vector in the direction of scattering, and hence we have $\hat{n}k_{p}=k_{\beta}$ where k_{β} is the wave-vector in the direction of scattering. In the above, β and b are the parameters of scattered electron.

If the velocity of the incident electron is very large, we can use the Born-Approximation (replacing $\psi_{\alpha a}(+)$ inside the integral sign in (178) by the free particle function $\phi_{\alpha a}$) and hence, we can write the asymptotic behaviour of $\psi_{\alpha a}(+)$ as follows:

$$\psi_{\alpha\alpha}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) \xrightarrow{r_2 \to \infty} \phi_{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2) + \sum_{b} \frac{\exp. (ik_{\alpha} r_2)}{r_2}$$

 $\times f(\mathbf{k}_{\beta}, b, \mathbf{k}_{\alpha}, a) w_{\alpha}(\mathbf{r}_{1})$

where the scattering amplitude $f(\mathbf{k}_{\beta}, b; \mathbf{k}_{\alpha}, a)$ is given by:

$$f(\mathbf{k}_{\beta}, h; \mathbf{k}_{\alpha}, a) = -\frac{1}{4\pi} \cdot \frac{2m}{\hbar^{2}} \iint \exp \left[-i\mathbf{k}_{\beta} \cdot \mathbf{r}'_{2} \right] w_{b}^{*} (\mathbf{r}'_{1})$$

$$H'(\mathbf{r}'_{1}, \mathbf{r}'_{2}) \times \phi_{\alpha a}(\mathbf{r}'_{1}, \mathbf{r}'_{2}) d^{3}r_{1}' d^{3}r'_{2}$$

$$= -\frac{2m}{4\pi\hbar^{2}} \iint \exp \left[-i\mathbf{k}_{\beta} \cdot \mathbf{r}'_{2} \right] w_{b}^{*} (\mathbf{r}'_{1}) H' (\mathbf{r}'_{1}, \mathbf{r}'_{2})$$

$$\times \exp \left[i\mathbf{k}_{\alpha} \cdot \mathbf{r}'_{2} \right] w_{a} (\mathbf{r}'_{1}) d^{3}r'_{1} d^{3}r'_{2}$$
or
$$f(\mathbf{k}_{\beta}, b; \mathbf{k}_{\alpha}, a) = -\frac{2m}{4\pi\hbar^{2}} \iint \exp \left[i \mathbf{K} \cdot \mathbf{r}'_{2} \right] w_{b}^{*} (\mathbf{r}'_{1}) H' (\mathbf{r}'_{1}, \mathbf{r}'_{2})$$

$$\times w_{a} (\mathbf{r}'_{1}) d^{3}r'_{1} d^{3}r'_{2},$$
where
$$\mathbf{K} = (\mathbf{k}_{\alpha} - \mathbf{k}_{\beta})$$
Or, deleting the primes and the primes and the primes and the primes are the second of the primes and the primes are the second of the primes are the second

Or, deleting the primes on the variables of integration, this can also be written as:

$$f(\mathbf{k}_{\beta}, b, \mathbf{k}_{\alpha}, a) = -\frac{2m}{4\pi \hat{\mathbf{n}}^2} \iint \exp \left[i \mathbf{K} \cdot \mathbf{r}_2\right] w_b^* (\mathbf{r}_1) H' (\mathbf{r}_1, \mathbf{r}_2)$$

This equation gives an exact several \mathcal{K} and $\mathcal{$

This equation gives an exact expression for the electron-atom scattering amplitude under Born-Approximation. However, we have neglected the exchange effects. Now we consider the specific example of the scattering of an electron from a hydrogen atom.

Electron Scattering from Hydrogen Atom. The interaction Hamiltonian in this case is given by:

$$H'(\mathbf{r}_1 \, \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_2 - \mathbf{r}_2|} - \frac{e^2}{r_2}$$
...(180)

Thus the scattering amplitude (179) can be written as:

$$f = -\frac{2m}{4\pi\hbar^2} \iint \exp. (i \, \mathbf{K} \cdot \mathbf{r}_2) \left(\frac{e^2}{|\mathbf{r}_2 - \mathbf{r}_1|} - \frac{e}{r_2} \right) w_b^*(r_1) w_a(\mathbf{r}_1) d^3 r_1 d^3 r_2$$

Frist we perform the integration with respect to r_2 . For it

$$\int \frac{\exp. (i \mathbf{K} \cdot \mathbf{r})}{r} d^3r = \frac{4\pi}{K} \int_0^\infty \sin Kr \, dr. \qquad \dots (182)$$

In order to evaluate this integral we add an integrating factor 'exp. $(-\alpha r)$ ' to the integrand and subsequently take the limit $\alpha \rightarrow 0$. Hence we have,

$$\int \frac{\exp \left(i \text{ K} \cdot \mathbf{r}\right)}{r} d^{3}r = \frac{4\pi \operatorname{Lim}}{K} \int_{0}^{\infty} \sin Kr \exp \left[-\alpha r\right] dr$$

$$= \frac{4\pi \operatorname{Lim}}{K} \operatorname{Im} \int_{0}^{\infty} \exp \left[-(\alpha - i K)r\right] dr$$

$$= \frac{4\pi}{K^{2}} \qquad ...(183)$$

Using this, we can now calculate the r_2 integral in 181. We have,

$$\int \frac{\exp \left[iK \cdot r_{2}\right]}{|r_{2}-r_{1}|} d^{3}r_{2} = \exp \left[iK \cdot r_{1}\right] \int \frac{\exp \left[iK \cdot (r_{2}-r_{1})\right]}{|r_{2}-r_{1}|} d^{3}r_{2}$$

$$= \exp \left[iK \cdot r_{1}\right] \int \frac{\exp \left(iK \cdot \rho\right)}{\rho} d^{3}\rho,$$

$$\text{where } \rho = r_{2}-r_{1}.$$

$$= \exp \left[iK \cdot r_{1}\right] \cdot \frac{4\pi}{K^{2}} \qquad \dots (184)$$

$$\int \exp \left[iK \cdot r_{2}\right] d^{3}r_{2} d\pi$$

and

$$\int \frac{\exp[iK.r_{9}]}{r_{2}} d^{3}r_{2} = \frac{4\pi}{K^{2}} \qquad ...(185)$$

Using eqns. (184) and (185) into (181) we get,

$$f = \frac{2me^2}{\hbar^2 K^2} \int (1 - \exp [i K \cdot r_1]) w_b^* (r_1) w_a (r_1) d^2 r_1$$
...(186)

For elastic scattering, the initial and the final state of the atom are the same, i.e., $w_a \equiv w_b$. Also, from energy conservation, $|\mathbf{k}_z| = |\mathbf{k}_\beta|$. Therefore, the scattering amplitude for the elastic scattering can be written as,

$$f_{e_1} = \frac{2me^2}{\hbar^2 K^2} \int (1 - \exp [iK \cdot r_1]) w_a^* (r_1) w_a (r_1) d^3 r_1 \dots (187)$$

For simplicity we consider the scattering of the electron from the ground state of hydrogen atom. Then,

$$w_a = \frac{1}{\sqrt{(\pi a_0^2)}} \exp[-r_1/a_0]$$

The first term in the integral of eqn. (187) gives unity due to the orthonormality of w_a (r_1) . The second itegral is,

$$\frac{1}{\pi a_0^3} \int \exp(i \mathbf{K} \cdot \mathbf{r}_1) \exp(-2r_1/a_0) d^3r_1$$

$$= \frac{4\pi}{\pi a_0^3 K} \int_0^\infty \sin K r_1 \exp_{-2 r_1/a_0} r_1 dr_1$$

$$= \frac{4\pi}{\pi a_0^3 K} \operatorname{Im}_{-1} \int_0^\infty \exp_{-1} \left[-\left(\frac{2}{a_0} - iK\right) r_1 \right] r_1 dr_1$$

$$= \frac{4\pi}{\pi a_0^3 K} \frac{K a_0^3}{4(1 + \frac{1}{4}a_0^2 K^2)^2} = (1 + \frac{1}{4}a_0^2 K^2)^{-2}$$

$$f_{\sigma l}(\theta) = \frac{2 me^2}{\hbar^2 K^2} \left[1 - (1 + \frac{1}{4}a_0^2 K^2)^{-2} \right] \qquad (188)$$

In the high energy case, for which the Born-approximation is the best approximation, ao K will be much larger than unity; and hence

$$f_{el}(\theta) \xrightarrow{K \text{ large}} \frac{2 me^2}{\hbar^2 K^2}$$
 ...(189)

In this case, Born approximation yields reliably good results for large angle scattering which is not true for the potential scattering. For potential scattering, by large angle we mean large momentum transfer and hence the Born-Approximation is not a goood approximation there.

For inelastic scattering, the initial state wa will be different from wb and hence the first term in the integrand of (186) gives zero because of the orthogonality of the unperturbed states of Thus, the atom.

$$f_{inci} = -\frac{2me^2}{\hbar^2 K^2} \int \exp \left[i \, \mathbf{K} \cdot \mathbf{r}_1\right] \, w_b^* \left(\mathbf{r}_1\right) \, w_a \left(\mathbf{r}_1\right) \, d^3\mathbf{r}_1 \qquad \dots (190)$$

As a simple example we consider the case when the ground state of the hydrogen atom (1s state) is excited to the state 2s (first excited state) due to collision with the electron. The scattering amplitude for this scattering is given by,

$$f_{inel} (1s \to 2s) = -\frac{2me^2}{\hbar^2 K^2} \int \exp \left[i K \cdot \mathbf{r}_1\right] w_{2s}^* (\mathbf{r}_1) w_{1s} (\mathbf{r}_1) d^3 r_1$$

$$= -\frac{2}{a_0 K^2} \int \exp \left[i K \cdot \mathbf{r}\right] w_{2s}^* (\mathbf{r}) w_{1s} (\mathbf{r}) d^3 r$$

$$\left(:: a_0 = \frac{\hbar^2}{me^2} \right)$$

For hydrogen atom we have

$$w_{1s} = \frac{1}{\sqrt{(\pi a_0^3)}} \exp \left[-r/a_0\right],$$
and
$$w_{2s} = \frac{1}{4\sqrt{(2^{\circ})} a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) \exp \left[-r/2a_0\right]$$

and

$$\frac{f_{inot}(1s \to 2s) = -\frac{2}{a_0 K^2} \cdot \frac{1}{a_0^3} \cdot \frac{1}{4\pi \sqrt{(2)}} \int \exp[iK \cdot \mathbf{r}]}{\times \left(2 - \frac{r}{a_0}\right) \exp[-\frac{3}{2} \cdot \frac{r}{a_0}] d^3r} \qquad \dots (191)$$
Now,
$$\int \exp[iK \cdot \mathbf{r}] \left(2 - \frac{r}{a_0}\right) \exp[-\frac{3}{2} \cdot \frac{r}{a_0}] d^3r$$

$$= \int \exp[iKr \cos \theta] \left(2 - \frac{r}{a_0}\right) \exp[-\frac{3r}{2a_0}] r^2 dr d (\cos \theta) d\phi$$

$$= \frac{2\pi \cdot 2}{K} \int \sin Kr \cdot \left(2 - \frac{r}{a_0}\right) \exp[-\frac{3r}{2a_0}] r dr$$

$$= \frac{4\pi}{K} \operatorname{Im} \cdot \int \exp[iKr] \left(2 - \frac{r}{a_0}\right) \exp[-\frac{3}{2} \cdot \frac{r}{a_0}] r dr$$

$$= \frac{4\pi}{K} \operatorname{Im} \cdot \left[\frac{2}{\left(\frac{3}{2a_0} - iK\right)^2} - \frac{2}{a_0\left(\frac{3}{2a_0} - iK\right)^3}\right]$$

$$= \frac{8\pi}{Ka_0} \operatorname{Im} \cdot \frac{\frac{3}{2} - iKa_0 - 1}{\left(\frac{3}{2a_0} - iK\right)^3}$$

$$= \frac{8\pi}{Ka_0} \frac{4K^3}{\left(\frac{9}{4a_0^2} + K^2\right)^3}$$

$$= \frac{8\pi}{Ka_0} \cdot \frac{4K^3 a_0^6}{\left(\frac{9}{4} + K^2a_0^2\right)^3}$$

$$\therefore f_{inot}(1s \to 2s) = \frac{-8\sqrt{(2)} a_0}{\left(\frac{9}{4} + K^2a_0^2\right)^3} \quad \dots (192)$$

9.12. EXCHANGE SCATTERING OF ELECTRON FROM HYDROGEN ATOM:

So far we have distinguished the incident and the atomic electrons in hydrogen atom. But in actual practice, due to the identity of the electrons, it is not possible to distinguish the two electrons after the scattering; i.e., we can not say that the electron which is scattered is the initial incident electron or it is an atomic electron. Therefore, we have to take the possibility of the exchange of the two electrons into consideration for electron-atom scattering.

Let us label the incident electron as e_1 and that the atomic electron as e_2 . If the electron e_1 is scattered, then the scattering is called the direct scattering and we have discussed it in detail in the preceding sub-section. However, if electron e_1 takes the place of the atomic electron e_2 and the electron e_3 is the scattered electron, we call the scattering as exchange scattering. In the exchange scattering, co-ordinates of the incident electron ' \mathbf{r}_1 ' and the coordinates of the atomic electron ' \mathbf{r}_2 ' are interchanged after the scattering has taken place, and hence the final state $\phi_{\beta b}$ for the exchange scattering can be written as:

$$\phi_{\beta b}^{exch}(\mathbf{r}_1, \mathbf{r}_2) = \exp[i\mathbf{k}_{\beta} \cdot \mathbf{r}_1] w_b(\mathbf{r}_2)$$
 ...(193)

Also, the asymptotic behaviour of $\psi_{\alpha\alpha}^{(+)}$ (\mathbf{r}_1 , \mathbf{r}_2) is given by:

$$\psi_{\alpha a}^{(+)} (\mathbf{r}_1, \mathbf{r}_2) \xrightarrow{---} \sum \frac{\exp[ik_{\beta} l_1]}{r_1} g(\mathbf{k}_{\beta}, b; \mathbf{k}_{\alpha}, a) w_b (\mathbf{r}_2)$$
...(194)

There is no unscattered part here, because the electron e_1 is captured in the atom. The scattering amplitude $g(k_{\beta}, b; k_{\alpha}, a)$ is given by:

$$g(\mathbf{k}_{\beta}, b \; ; \; \mathbf{k}_{\alpha}, a) = \frac{-2m}{4\pi\hbar^{2}} \iint \phi_{\beta b}^{exch} * (\mathbf{r}_{1}, \mathbf{r}_{2}) \; H' \; (\mathbf{r}_{1}, \mathbf{r}_{2}) \; \psi_{\alpha a}^{(+)} \; (\mathbf{r}_{1}, \mathbf{r}_{2}) \; d^{3}r_{1}d^{3}r_{2}$$

$$= \frac{-2m}{4\pi\hbar^{2}} \iint \exp \left[-i\mathbf{k}_{\beta} \cdot \mathbf{r}_{1}\right] w_{b}^{*} \; (\mathbf{r}_{2}) \; H' \; (\mathbf{r}_{1}, \mathbf{r}_{2}) \; \psi_{\alpha a}^{(+)} \; (\mathbf{r}_{1}, \mathbf{r}_{2}) \; d^{3}r_{1} \; d^{3}r_{2}$$

$$\dots (195)$$

Now, due to the identical nature of the electrons, it is not possible to label them, and according to the Pauli's exclusion principle, the total wavefunction $\psi^{(+)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{s}_1, \mathbf{s}_2)$ should be properly symmetrized. Since the electrons are fermions, the total wavefunction should be antisymmetric. In the non-relativistic limit, the total wavefunction can be written as:

$$\psi^{(+)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{s}_1, \mathbf{s}_2) = \psi^{(+)}(\mathbf{r}, \mathbf{r}_2) \chi^{(+)}(\mathbf{s}_1, \mathbf{s}_2), \dots (196)$$

where $\psi^{(+)}$ $(\mathbf{r}_1, \mathbf{r}_2)$ is the space part and $\chi^{(+)}$ $(\mathbf{s}_1, \mathbf{s}_2)$ is the spin part of the total wavefunction. Since $\chi^{(+)}$ $(\mathbf{s}_1, \mathbf{s}_2)$ describes two spinhalf particles (electrons), we can have either a singlet state $(\downarrow\uparrow)$ or a triplet state $(\uparrow\uparrow)$. The singlet state is given by:

$$\chi_{sing}^{(+)}(s_1, s_2) = \frac{1}{\sqrt{(2)}} \left\{ \alpha(1) \beta(2) - \alpha(2) \beta(1) \right\} \dots (197)$$

which is antisymmetric. Thus to make the total wavefunction anti-symmetric, we symmetrize the space part as:

$$\psi_{sym}(\cdot) (\mathbf{r}_1, \mathbf{r}_2) = \psi_{\alpha\alpha}(+) (\mathbf{r}_1, \mathbf{r}_2) + \psi_{\alpha\alpha}(+) (\mathbf{r}_2, \mathbf{r}_1) \dots (198)$$

First function on the right hand side corresponds to the direct scattering and the second one corresponds to the exchange scattering. Asymptotic behaviour of the symmetrized wavefunction (198) can be written as:

$$\psi_{sym}^{(+)} (\mathbf{r}_1, \mathbf{r}_2) \xrightarrow[r_1 \to \infty]{} \phi_{\alpha a} (\mathbf{r}_1, \mathbf{r}_2) + \sum_{b} \frac{\exp [ik_{\beta} r_1]}{r_1} (f+g) w_b (\mathbf{r}_2) \dots (199)$$

Thus the scattering amplitude in the singlet state is the sum of the direct and the exchange scattering amplituds, and hence the scattering cross-section for singlet state is given by:

$$\sigma_{sing} = \frac{k_{\beta}}{k_{\alpha}} |f+g|^2$$
 ...(200)

The triplet state is given by:

$$\chi^{(+)}_{trip} (s_1, s_2) = \begin{cases} \alpha(1) \alpha(2) \\ \beta(1) \beta(2) \\ \frac{1}{\sqrt{(2)}} \left\{ \alpha(1) \beta(2) + \alpha(2) \beta(1) \right\}, \end{cases} \dots (201)$$

i.e., all the triplet states are symmetric. Thus to make the total wavefunction antisymmetric, we make the space part antisymmetric

$$\psi_{antisym.}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{\alpha a}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) - \psi_{\alpha a}^{(+)}(\mathbf{r}_2, \mathbf{r}_1)$$
 ...(202)

In this case, scattering amplitude will be (f-g) and hence the scattering cross-section in triplet state is given by:

$$\sigma_{trip} = \frac{k_{\beta}}{k_{\alpha}} |f - g|^2$$
 ...(203)

Equations (200) and (203) give the differential scattering cross-sections, including the exchange effect. Total differential scattering cross-section is the sum of σ_{sing} , and σ_{trip} , with their proper statistical weight factors:

$$\left(\frac{d\sigma}{d\Omega}\right)_{tot.} = \frac{1}{4} \sigma_{sing.} + \frac{3}{4} \sigma_{trip.} \qquad \dots (204)$$

In order to evaluate (204), we should calculate f and g. The direct scattering amplitude f has already been calculated [see eqn. (186)]. For g, we have from eqn. (195) that:

$$g = -\frac{2m}{4\pi\hbar^2} \iint \exp \left\{-i\mathbf{k}_{\beta} \cdot \mathbf{r}_1\right\} w_b^* (\mathbf{r}_2) H'(\mathbf{r}_1, \mathbf{r}_2) \psi_{\alpha\alpha}^{(+)} (\mathbf{r}_1, \mathbf{r}_2) d^3r_1 d^3r_2$$

To calculate g, we make use of an approximation, known as the Born-Oppenheimer-Approximation In this approximation, we replace $\psi_{\alpha\alpha}^{(+)}$ (\mathbf{r}_1 , \mathbf{r}_2) by the state $\Phi_{\alpha\alpha}$ (\mathbf{r}_1 , \mathbf{r}_2); the unperturbed wavefunction before scattering.

$$g = -\frac{1}{4\pi} \cdot \frac{2m}{\hbar^2} \iint \exp \left\{ -i\mathbf{k}_{\beta} \cdot \mathbf{r}_1 \right\} w_b^* (\mathbf{r}_2) H' (\mathbf{r}_1, \mathbf{r}_2) \times \exp \left\{ i\mathbf{k}_{\alpha} \cdot \mathbf{r}_2 \right\} w_a (\mathbf{r}_1) d^3 r_1 d^3 r_2 \dots (205)$$

The initial and the final states of the atom are not now orthogonal to each other. Due to this, a number of discrepancies are incorporated into the Born-Oppenheimer-Approximation:

- (i) If we add a constant C to the interaction part of the Hamiltonian, $H'(\mathbf{r}_1, \mathbf{r}_2)$, the scattering cross-section changes; while on physical grounds there should not be any change.
- (ii) The interaction potential $H'(r_1, r_2)$ is given by $\frac{e^2}{r_{12}} \frac{e^2}{r_2}$ before the collision; and by $\frac{e^2}{r_{12}} \frac{e^2}{r_1}$ after the collision.

Using these two forms for H' we get two different values of g. Since we do not know that which form of H' is to be used, there is produced a discrepancy in the calculation of g. This defect is known as the postprior discrepancy.

(iii) The cross-section obtained in this approximation violates the maximum cross-section theorem.

Due to these discrepancies, Born Oppenheimer Approximation is not a popular approximation for evaluating 'g'. We, therefore, use another better approximation by *Ochkur*. In this approximation, g is expanded in the inverse powers of k_{α} and the leading term only is retained. We write,

$$g \equiv g_{n_0} + g_{\theta\theta}$$
; ...(206)

. .

where g_{ec} is the contribution due to electron-electron interaction and g_{nc} is the contribution due to nuclear interaction. We have,

$$g_{ez} = -\frac{2me^2}{4\pi\hbar^2} \iint \exp \left\{ -i\mathbf{k}_{\beta} \cdot \mathbf{r}_1 \right\} w_b^* (\mathbf{r}_2) \frac{1}{r_{12}} \exp \left\{ i\mathbf{k}_z \cdot \mathbf{r}_2 \right\} \times w_a (\mathbf{r}_1) d^3 r_1 d^3 r_2 \dots (207)$$

Now,

$$\frac{1}{r_{12}} = \frac{1}{2\pi^2} \int \frac{\exp. \{iS.(r_2 - r_1)\}}{S^2} d^3S.$$

:4

Therefore,

$$g_{e3} = -\frac{2me^{2}}{8\pi^{3}\hbar^{2}} \iiint \frac{1}{S^{2}} \exp \left\{ iS.(\mathbf{r}_{2} - \mathbf{r}_{1}) + i\mathbf{k}_{\alpha}.(\mathbf{r}_{2} - \mathbf{r}_{1}) + i\mathbf{k}_{\alpha}.\mathbf{r}_{1} - i\mathbf{k}_{\beta}.\mathbf{r}_{1} \right\}$$

$$\times w_{b}^{*} (\mathbf{r}_{2}) w_{\sigma} (\mathbf{r}_{1}) d^{3}r_{1} d^{3}r_{2} d^{3}S \qquad ...(208)$$

$$= -\frac{1}{8\pi^{3}} \cdot \frac{2me^{2}}{\hbar^{2}} \iiint \frac{1}{S^{2}} \exp \left\{ i (S + \mathbf{k}_{\alpha}).(\mathbf{r}_{2} - \mathbf{r}_{1}) + i\mathbf{K}.\mathbf{r}_{1} \right\}$$

$$\times w_{b}^{**} (\mathbf{r}_{2}) w_{a} (\mathbf{r}_{1}) d^{3}r_{1} d^{3}r_{2} d^{3}S.$$

First we consider the integral

$$I = \int \frac{\exp\left(\frac{i\left(S + k_{\alpha}\right) \cdot \left(r_{2} - r_{1}\right)}{S^{2}}\right) d^{3}S}{S^{2}}.$$

To evaluate it, we put $(S + k_z) = p$. Then

$$I = \int \frac{\exp\left\{i\mathbf{p}\cdot(\mathbf{r}_2 - \mathbf{r}_1)\right\}}{|\mathbf{p} - \mathbf{k}_z|^2} d^3p$$

The integrand in the above integral is an oscillating function of p. If p is large, oscillations will be rapid and hence the integral will vanish. If p is small, the integrand will be varying slowly and the integral won't vanish. For very small values of p, we can neglect it in comparison with k_{α} and hence we can write,

$$I \frac{1}{k_{\alpha}^{2}} \int \exp \left\{ i \mathbf{p} \cdot (\mathbf{r}_{2} - \mathbf{r}_{1}) \right\} d^{3}p = \frac{1}{k_{\alpha}^{2}} (2\pi)^{3} \delta^{3} (\mathbf{r}_{2} - \mathbf{r}_{1})$$

$$\therefore g_{eo} = -\frac{1}{8\pi^{3}} \cdot \frac{2me^{2}}{\hbar^{2}} \cdot (2\pi)^{3} \cdot \frac{1}{k_{\alpha}^{2}} \iint \delta^{3} (\mathbf{r}_{2} - \mathbf{r}_{1}) \exp \left\{ i \mathbf{K} \cdot \mathbf{r}_{1} \right\}$$

$$\times w_{b}^{*} (\mathbf{r}_{2}) w_{c} (\mathbf{r}_{1}) \cdot d^{3}r_{1} d^{3}r_{2}$$

$$= -\frac{2me^2}{\hbar^2} \cdot \frac{1}{k_{\alpha}^2} \int \exp \{i\mathbf{K} \cdot \mathbf{r}_2\} w_b^* (\mathbf{r}_2) w_a (\mathbf{r}_2) d^3 r_2$$

Also, it can very easily be seen that

$$g_{nc} \xrightarrow{\text{large } k} \frac{1}{k_{\alpha}^{6}}$$

Now, keeping only the leading term in g, we get:

g (Ochkur) =
$$-\frac{2me^2}{\hbar^2} \cdot \frac{1}{k_{\alpha}^2} \int \exp \{i\mathbf{K} \cdot \mathbf{r}_2\} w_b^* (\mathbf{r}_2) w_a (\mathbf{r}_2) d^3 r_2$$
 ...(209)

Clearly, there is no post-prior discrepancy in the Ochkur approximation.

The direct scattering amplitude f in the Born-Approximation is given by:

$$f = \frac{1}{4\pi} \cdot \frac{2me^2}{\hbar^2} \cdot \frac{4\pi}{K^2} \int (1 - \exp \{i\mathbf{K} \cdot \mathbf{r}_2\}) w_b^* (\mathbf{r}_2) w_a (\mathbf{r}_2) d^3 r_2$$

$$= \frac{2me^2}{\hbar^2 K^2} \left[\delta_{ba} - \int \exp \{i\mathbf{K} \cdot \mathbf{r}_2\} w_b^* (\mathbf{r}_2) w_a (\mathbf{r}_2) d^3 r_2 \right]$$

Using this, we can write (209) as:

g (Ochkur) =
$$\frac{K^2}{K_{\alpha}^2} \left[f - \frac{2me^2}{\hbar^2 K^2} \delta_{ba} \right]$$
 ...(210)

For inelastic scattering, $a \neq b$. Therefore, $\delta_{ba} = 0$ and hence we have

g (Ochkur) =
$$\frac{K^2}{K_{\alpha^2}}.f.$$
 ...(211)

For elastic scattering, a=b and hence $\delta_{ba}=1$. Therefore,

g (Ochkur) =
$$\frac{K^2}{K_{\alpha}^2} \left[f - \frac{2me^2}{\hbar^2 K^2} \right]$$
 ...(212)

Now, for elastic scattering of electron with hydrogen atom,

$$f = \frac{2me^2}{\hbar^2 K^2} \left[1 - \left(1 + \frac{1}{4} a_0^2 K^2 \right)^{-2} \right] = \frac{2a_0 \left(8 + K^2 a_0^2 \right)}{\left(4 + K^2 a_0^2 \right)^2}.$$

:.
$$g(\text{Ochkur}) = -\frac{32}{k_{\alpha}^2 (4 + K^2 a_0^2)^2}$$
 ...(213)

Hence the elastic differential scattering cross-section for the electron hydrogen atom scattering with the exchange effects taken into account, is given by:

$$\left(\frac{d\sigma}{d\Omega}\right)_{tot} = \frac{1}{4} |f+g(Ochkur)|^2 + \frac{3}{4} |f-g(Ochkur)|^2 \dots (214)$$

The results of eqn. (214) are in very good agreement with the observed results for large values of the energy of the incident electron. However, for low energy incident electron, argument is not very good.

"Problems".

Problem 1. Obtain the Rutherford cross section for the scattering of charged particles by the Coulomb field of nuclei, using the partial wave method.

Sol. The Coulomb potential for the scattering of particle of charge ze from the nucleus of charge Ze is given by

$$V(r) = \frac{Zze^2}{r}.$$
 ...(i)

It is clear that the potential V(r) does not fall faster than 1/rat asymptotic distances, which is a necessary condition for the partial wave method to be applicable. Even then the partial wave analysis gives correct results in this case. The Coulomb potential is an exceptional scatterer in this respect.

The Schroedinger equation for (i) can be written as,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{Zze^2}{r} - \frac{\hbar^2k^2}{2m}\right)\psi_c(\mathbf{r}) = 0$$

$$mZze^2$$

or
$$(\nabla^2 + k^2 - 2nk/r) \psi_c(\mathbf{r}) = 0$$
; $n = \frac{mZze^8}{\hbar^2 k}$...(ii)

The subscript c for ψ specifies it for Coulomb field. To solve Eqn. (ii) for ψe and subsequently to get its asymptotic behaviour, we use the parabolic coordinates ξ , η , ϕ ; defined in terms of spherical polar coordinates as

$$\begin{cases}
\xi = r - z = r \left(1 - \cos \theta\right) \\
\eta = (r + z) = r \left(1 + \cos \theta\right)
\end{cases} \dots \text{(iii)}$$

$$\phi = \phi$$

In terms of the parabolic co-ordinates,

Since the potential V(r) is spherically symmetric, therefore, the solution ψ_c will be independent of ϕ and hence using (iv), we can write eqn. (ii) in terms of the parabolic co-ordinates as:

write eqn. (ii)
$$\frac{1}{2k}\left(\frac{\partial}{\partial \xi}\left(\xi \frac{\partial}{\partial \xi}\right) + \frac{\partial}{\partial \eta}\left(\eta \frac{\partial}{\partial \eta}\right)\right) + k^2 - \frac{4nk}{\xi + \eta}\right]\psi_c = 0.$$
 ...(v)

We are interested to solve (v) under the asymptotic boundary condition

dition
$$\psi_{c} \xrightarrow{\longrightarrow} e^{ikz} \left(1 + \frac{f(\theta)}{r} e^{ik \cdot (r-z)} \right)$$

$$= e^{ikz} f(\xi); f(\xi) = \left(1 + \frac{f(\theta)}{r} e^{ik\xi} \right) \qquad \{ : \xi = r - z \}.$$

$$= e^{ikz} f(\xi); f(\xi) = \left(1 + \frac{f(\theta)}{r} e^{ik\xi} \right) \qquad \text{differential}$$

Substituting this into (v), we get the following differential equation for $f(\xi)$,

$$\xi \frac{d^2f}{d\xi^2} + (1 - ik\xi) \frac{df}{d\xi} - nkf = 0.$$
 ...(vi)

This equation is exactly of the form of confluent hypergeometric equation

$$z \frac{d^2F}{dz^2} + (b-z) \frac{dF}{dz} - aF = 0;$$
which is the configuration (vii)

the solution of which is the confluent hypergeometric function

$$F(a, b, z) = \sum_{s=0}^{\infty} \frac{\Gamma(a+s) \Gamma(b)}{\Gamma(a) \Gamma(b+s)} \cdot \frac{z^{s}}{s!} = 1 + \frac{a}{b} z + \frac{a(a+1)}{b(b+1)2!} z^{2} + \dots$$

Comparing (vii) with (vi), we see that a=-in, b=1 and $z-ik\xi$(viii)

Thus the solution of (vi) can be written as

 $f(\xi)=cF(-in, 1, ik\xi)$; with c as an arbitrary constant.

$$\psi_c = c \cdot e^{ikz} F(-in, 1, ik\xi). \qquad \dots (ix)$$

In order to find its asymptotic behaviour, we need the asymptotic behaviour of the confluent hypergeometric function.

The confluent hypergeometric equation is a second order differential equation and hence the solution of it is consisted of two functions W_1 (a, b, z) and W_2 (a, b, z). Thus the general solution is given by

$$F(a, b, z) = W_1(a, b, z) + W_2(a, b, z),$$
 ...(x)

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with,

$$W_1(a, b, z) = \frac{\Gamma(b)}{\Gamma(b-a)} (-z)^{-a} g(a, a-b+1, -z),$$

$$W_2(a, b, z) = \frac{\Gamma(b)}{\Gamma(a)} e^z \cdot z^{a-b} g(1-a, b-a, z)$$
, and

$$g(\alpha, \beta, z) \xrightarrow{r \to \infty} 1 + \frac{\alpha\beta}{z! \cdot 1!} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{z^2 \cdot 2!} + \dots$$

$$: W_1(a, b, z) \xrightarrow{} \frac{\Gamma(b)}{z \to \infty} \frac{\Gamma(b)}{\Gamma(b-a)} (-z)^{-a} \left\{ 1 + \frac{a(a-b+1)}{-z} \right\}, \text{ and}$$

$$W_2(a, b, z) \sim \rightarrow \frac{\Gamma(b)}{\Gamma(a)} \cdot e^z \cdot z^{a-b}$$

Therefore,

$$F(a, b, z) \xrightarrow{r \to \infty} \frac{\Gamma(b)}{\Gamma(b-a)} \cdot (-z)^{-a} \left\{ 1 + \frac{a(a-b+1)}{-z} \right\}$$

$$+ \frac{F(b)}{F(a)} e^{z} \cdot z^{a-b}. \qquad (xi)$$

Using (xi), we can write

Using (x1), we can write

$$\psi_{c} \underset{r \to \infty}{\longrightarrow} c \cdot e^{ikz} \left\{ \frac{1}{\Gamma(1+in)} \left(-ik\xi \right)^{in} \left[1 + \frac{(-in)(-in)}{(-ik\xi)} \right] \right. \\
\left. + \frac{1}{\Gamma(-in)} e^{ik\xi} \left(ik\xi \right)^{-in-1} \right\} \\
= \frac{ce^{n\pi/2}}{\Gamma(1+in)} \left\{ \exp \cdot \left\{ i \mid [kz+nl_nk(r-z)] \right\} \left[1 + \frac{n^2}{ik(r-z)} \right] \right. \\
\left. + \frac{\Gamma(1+in)}{\Gamma(-in)} \cdot \frac{1}{2ikr\sin^2\frac{\theta}{2}} \exp \cdot \left\{ i \left[kr-nl_n\left(2kr\sin^2\frac{\theta}{2} \right) \right] \right\} \right\} \\
\left\{ \cdot \cdot \left(k\xi \right)^{in} = \exp \cdot \left[inl_n\left(k\xi \right) \right] ; \left(-i \right)^{in} = (i)^{-in} = e^{n\pi/2} ; \\
\xi = r - z = r\left(1 - \cos\theta \right) = 2r\sin^2\frac{1}{2}\theta \right\} \\
= \frac{ce^{n\pi/2}}{\Gamma(1+in)} \cdot \left\{ \exp \cdot \left\{ i \left[kz+nl_n k(r-z) \right] \right\} \left[1 + \frac{n^2}{ik(r-z)} \right] \right. \\
\left. + \frac{f_c(\theta)}{r} \exp \cdot \left\{ i \left[kr-nl_n 2kr \right] \right\} \right\} \dots (xii)$$
with
$$\frac{f_c(\theta)}{r} = \frac{\Gamma(1+in)}{\Gamma(-in)} \cdot \frac{1}{2ikr\sin^2\frac{\theta}{2}} \cdot \exp \cdot \left\{ -inl_n\left(\sin^2\frac{\theta}{2} \right) \right\} \cdot \dots (xiii)$$

From the definition, $\Gamma(1-z) = -z \Gamma(-z)$. Therefore, $F(-in) = \frac{\Gamma(1-in)}{in}$

Using this, we have from (xiii) that

$$f_c(\theta) = \frac{n}{2k \sin^2 \frac{\theta}{2}} \cdot \frac{\Gamma(1+in)}{\Gamma(1-in)} \cdot (-1) \cdot \exp \left\{-inl_n\left(\sin^2 \frac{\theta}{2}\right)\right\}.$$

Now,
$$(-1)=e^{i\pi}$$
 and $\frac{\Gamma(1+in)}{\Gamma(1-in)}=e^{2i\eta_0}$ with $\eta_0=\text{Arg. }\Gamma(1+in)$

$$\therefore f_c(\theta) = \frac{n}{2k \sin^2 \frac{\theta}{2}} \cdot \exp\left\{-inl_n\left(\sin^2 \frac{\theta}{2}\right) + in + 2i\eta_0\right\} \dots (xiv)$$

The fc term on the right hand side of (xii) represents the outgoing scattered wave, because it is the only term depending on the factor $\frac{e^{ik\mathbf{r}}}{r}$. The first term, therefore, represents an incident "plane wave". Both the incident and the scattered wave are distorted at infinite distances by logarithmic phase factors. The differential scattering cross-section is given by

$$\frac{d\sigma_c(\theta)}{d\Omega} = |f_o(\theta)|^2 = \left|\frac{n}{2k \sin^2 \theta/2}\right|^2 = \left(\frac{Zze^2}{2mv^2}\right)^2 \operatorname{cosec}^4 \frac{\theta}{2}. \quad ...(xv)$$

This is exactly the formula obtained by Rutherford from classical dynamics.

Problem 2. Use the partial wave method to calculate the total scattering cross-section in the limiting cases of very low and very high incident energy for the scattering of a particle from the hard sphere potential of radius a,

$$V(r) = \begin{cases} +\infty & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

Compare the results with the corresponding classical results.

The boundary conditions for the hard sphere potential requires that the radial wavefunction $R_1(r)$ should vanish at r=a. Therefore,

$$\beta_{l} = \frac{a}{R_{l}} \cdot \frac{dR_{l}}{dr} \bigg|_{r \to a} = \infty, \qquad \dots (i)$$

because $\frac{dR_l}{dr}$ is infinite for r=a as explained below:

Since R_l has to vanish at r=a, due to the boundary condition, it should cross the r-axis at this point, because R_l is finite within the potential range. Thus the slope $\frac{dR_l}{dr}$ of R_l at r=a is finite,

which can easily be seen from the adjoining (fig. 14).

Now,

$$S_{i} = \frac{1}{ka(j_{i}^{2} + n_{i}^{2})}$$

and
$$\Delta_{l}=ka\frac{j_{l}'j_{l}+n_{l}'n_{l}}{j_{l}^{2}+n_{l}^{2}},$$

are finite. Hence we have

$$\tan \tau_i = \frac{S_I}{\beta_i - \Delta_I} = 0 \quad \text{or} \quad \tau_i = 0. \quad \dots \text{(ii)}$$

Therefore, from equation (53), we see that $\delta_i = \xi_i$, where ξ_i is given by

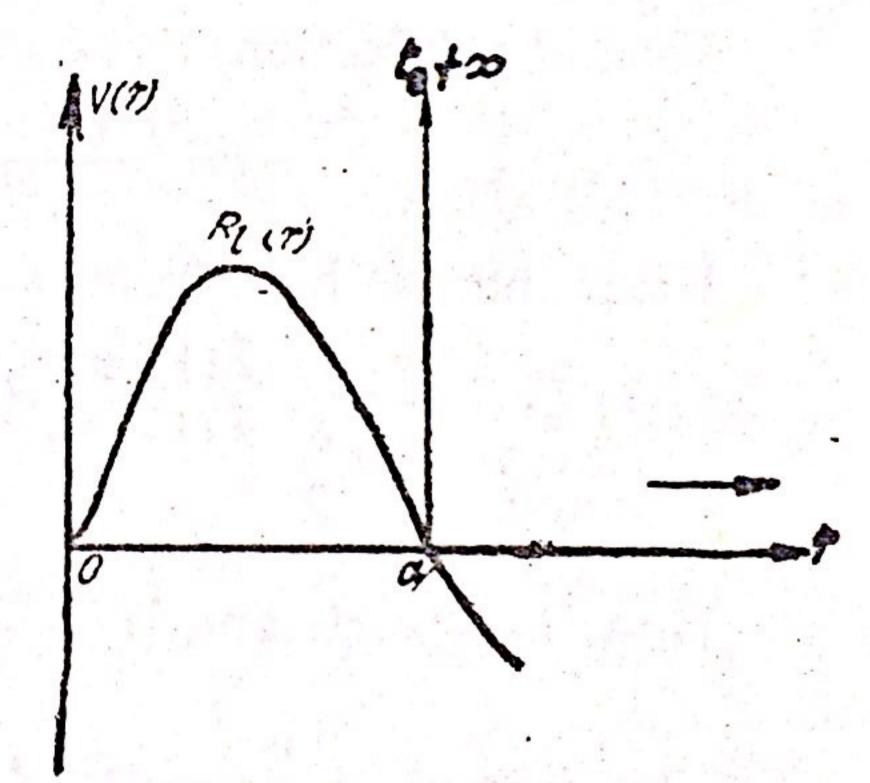


Fig. 14

or

w

*

$$-\frac{j_{l}-i\eta_{l}}{j_{l}+i\eta_{l}} = e^{2i\xi_{l}} \quad \text{or} \quad \tan \xi_{l} = \frac{j_{l}(ka)}{\eta_{l}(ka)}$$

$$\xi_{l} = \tan^{-1}\left\{\frac{j_{l}(ka)}{\eta_{l}(ka)}\right\}.$$

$$\delta_{l} = \tan^{-1}\left\{\frac{j_{l}(ka)}{\eta_{l}(ka)}\right\}. \quad \dots \text{(iii)}$$

This gives the 1th partial wave phase, shift. From it, we have

$$\sin \delta_{l} = \frac{j_{l} (ka)}{[j_{l}^{2} (ka) + n_{l}^{2} (ka)]^{12}} \cdot ...(iv)$$

Hence the total scattering cross-section is given by

$$\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \frac{j_l^2(ka)}{j_l^2(ka) + n_l^2(ka)}.$$

We now consider the cases of low and high energy incident particle.

(I) For low energy, k will be very-very small and hence ka < < 1. In this limit

$$j_l(ka) \approx \frac{(ka)^l}{(2l+1)!!}$$
 and $n_l(ka) \approx \frac{-(2l-1)!!}{(ka)^{l+1}}$...(vi)

From (vi), we see that $j_i(ka)$ wil be much smaller that $\eta_i(ka)$ for ka < < 1. Hence we can neglect it in the denominator in (v). Thus we get

$$\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \frac{(ka)^{4i+2}}{[(2l+1)!! (2l-1)!!]^2} \dots (vii)$$

For small energy (ka < < 1), all the phase shifts vanishes except l=0. Therefore, we keep only l=0 term in (vii) for this case, to get

(II) In the high energy limit (ka > > 1), j_i (ka) and $u_i(ka)$ can be replaced by their asymptotic forms

$$j_{l}(ka) \rightarrow \frac{\sin\left(ka - \frac{l\pi}{2}\right)}{ka},$$

$$j_{l}(ka) \rightarrow \frac{\cos\left(ka - \frac{l\pi}{2}\right)}{ka}.$$

$$\eta_{l}(ka) \rightarrow \frac{ka}{ka}$$

Using these values into (v), we see that in this case,

$$\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\left(ka - \frac{l\pi}{2}\right) = \frac{4\pi}{k^2} \cdot \frac{k^2a^2}{2} = 2\pi a^2 \cdot \dots (ix)$$

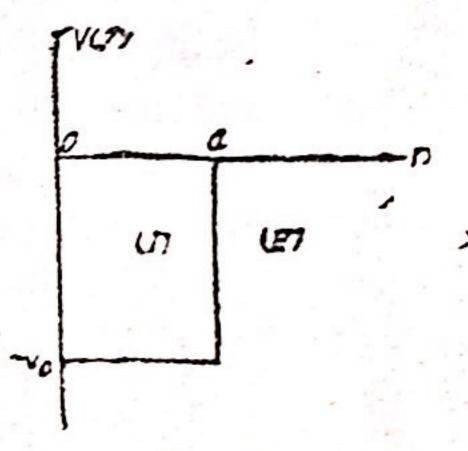
The classical mechanics gives $\sigma_{tot} = \pi a^2$. Thus the value (ix) is two times the classical value, whereas, in high energy limit we expect the classical result. What is the reason for this anamoly? The most important reason for it is that for high energies; the wavelength will be very small, and as our potential becomes infinity, suddenly at r=a, it won't be slowly varying within one wavelength. Thus the transition from Quantum Mechanics to Classical Mechanics is not possible for which the potential should be slowly varying within one wavelength.

Problem 3. Find out the s-wave scattering cross section for the scattering from the spherically symmetric square well potential of attractive nature,

$$V(r) = \begin{cases} --V_0 & for \quad r \leq a \\ 0 & for \quad r > a \end{cases}$$

Sol. Inside the potential, in region (I), the radial part of the Schroedinger equation is

$$\left(\frac{d^2}{dr^2} + \frac{2 d}{r dr} + \frac{2mV_0}{\hbar^2} + k^2 - \frac{l(l+1)}{r^2}\right) R_l(r) = 0.$$
(i)



Outside the potential well, in region (II), the radial equation is

Fig. 15.

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2}\right) R_1(r) = 0.$$
 ...(ii)

The regular solution of this eqn. is the Bessel's function $j_i(kr)$.

Putting $\alpha^2 = \left(k^2 + \frac{2mV_0}{\hbar^2}\right)$, the equation inside the potential well can be written as

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \alpha^2 - \frac{l(l+1)}{r^2}\right)R_1(r) = 0. \qquad \dots \text{(iii)}$$

Comparing it with (ii), we see that its reagular solution can be written as

$$R_l(r)=j_l(\alpha r)$$
 ...(iv)

$$\beta_{i} = \frac{a}{R_{i}(r)} \frac{dR_{i}(r)}{dr} \Big|_{r-a} = \frac{\alpha a j_{i}'(\alpha a)}{j_{i}(\alpha a)} \dots (v)$$

4.

For s-wave scattering, energy of the particle should be very small (ka < < 1) and only the l=0 partial wave will contribute. Therefore, we have

$$\beta_0 = \alpha a \frac{j_0'(\alpha a)}{j_0(\alpha a)} = (\alpha a \cot \alpha a - 1) \left\{ : j_0(x) = \frac{\sin x}{x} \right\}$$

At the end of Section 4 we have seen that for very low energy scattering, the phase shift is given by:

$$\delta_{l} = \frac{(ka)^{2l+1}}{(2l+1)!!} \cdot \frac{l-\beta_{l}}{\beta_{l}+l+1}$$

$$\vdots \quad \delta_{0} = -ka \frac{\beta_{0}}{\beta_{c}+1} = -ka \frac{(\alpha a \cot \alpha a - 1)}{(\alpha a \cot \alpha a - 1 + 1)}$$

$$= -ka + \frac{k}{\alpha} \tan \alpha a \qquad \dots (vi)$$

Thus the S-wave scattering cross section is given by

$$\sigma_0 = \frac{4\pi}{k^2} \, \delta_0^2 = 4\pi a^2 \, \left(1 - \frac{\tan \alpha a}{\alpha a} \right)^2 \, \dots \text{(vii)}$$

Problem 5. The potential energy for scattering of an electron by an atom can be represented approximately by the 'screened' Coulomb potential

$$V(r) = \frac{-Ze^2}{r}e^{-r/a} \qquad ...(i)$$

where 'a' is the screening radius.

Show that, in the first Born-Approximation, the scattering amplitude is

$$f(\theta) = \frac{2mZe^2a^2}{\hbar^2(1+K^2a^2)}$$
; $K=2k \sin \frac{\theta}{2}$...(ii)

Establish the criteria for validity of the Born-approximation in this case.

Sol. In the first Born-approximation, the scattering amplitude is given by Eqn. (171):

$$f(\theta) = -\frac{2m}{\hbar^2 K} \int_0^\infty r \sin Kr \ V(r) \ dr, \qquad \dots \text{(iii)}$$

where K=k-k',

$$K^2 = 2k^2 - 2k^2 \cos \theta$$

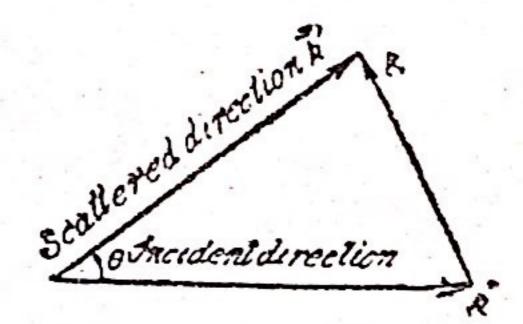
$$= 2k^2 (1 - \cos \theta)$$

$$= 4k^2 \sin^2 \theta/2$$

Hence, $K=2k \sin \theta/2$

Putting the value of V(r) from (i) into (iii) we obtain

$$f(\theta) = \frac{2mZe^2}{\hbar^2 K} \int_0^\infty \sin K \, r \, e^{-r/a} \, dr$$



Fnr elastic scattering

$$|\overrightarrow{k}| \overrightarrow{k'}| = k$$
Fig 16.

$$= \frac{2mZe^{2}}{\hbar^{2}K} Im. \int_{0}^{\infty} e^{iKr - r/a} dr$$

$$= \frac{2mZe^{2}}{\hbar^{2}K} Im. \frac{1}{\left(\frac{1}{a} - iK\right)} = \frac{2mZe^{2}}{\hbar^{2}K} \cdot \frac{K}{\left(\frac{1}{a^{2}} + K^{2}\right)}$$

$$= \frac{2mZe^{2}a^{2}}{\hbar^{2}(1 + a^{2}K^{2})} \qquad ...(iv)$$

From it, the differential scattering cross section is given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4m^2Z^2e^4a^4}{\hbar^4(1+a^2K^2)^2}, \dots (v)$$

and hence the total scattering cross-section is given by

$$\sigma_{tot} = 2\pi \int_{0}^{\pi} |f(\theta)|^{2} \sin\theta d\theta$$

$$= 2\pi \int_{0}^{2k} \frac{4m^{2}Z^{2}e^{4}a^{4}}{\hbar^{4} (1+a^{2}K^{2})^{2}} \frac{KdK}{k^{2}} \left\{ \vdots \quad K^{2} = 2k^{2} (1-\cos\theta) \right\}$$

$$= \frac{8\pi m^{2}Z^{2}e^{4}}{\hbar^{4}k^{2}} \cdot \frac{1}{2a^{2}} \left[\frac{-1}{1+a^{2}K^{2}} \right]_{0}^{2k}$$

$$= \frac{16\pi m^{2}Z^{2}e^{4}a^{4}}{\hbar^{4} (1+4k^{2}a^{2})} \qquad ...(vi)$$

To establish the criteria for validity, we have the validity condition. Eqn. (174) as:

$$\frac{m}{\hbar^2 k} \Big| \int_0^\infty (e^{2ikr} - 1) V(r) dr \Big| < 1$$
 ...(vii)

Thus we have to evaluate the integral

$$I = -\int_0^\infty (e^{2ikr} - 1) \frac{e^{-r/a}}{r} dr = -\int_0^\infty (e^{2ikr} - 1) \frac{e^{-ar}}{r} dr; \alpha = \frac{1}{a}.$$

Now,

$$\frac{dI}{d\alpha} = \int_0^\infty (e^{-2ikr} - 1) e^{-\alpha r} dr$$

$$= -\frac{1}{\alpha} + \frac{1}{\alpha - 2ik}$$

$$\therefore I=\ln(\alpha-2ik)-\ln\alpha+C;$$

where C is the constant of integration. To find the value of C we use the condition that the limit $\alpha \to \infty$; the integral $I \to 0$. Therefore,

$$0 = \ln\left(1 - \frac{2ik}{\alpha}\right) + C = \ln 1 + C = C$$

$$\therefore I = \ln\left(1 - \frac{2ik}{\alpha}\right) = \ln\left(1 - 2ika\right) \qquad \dots \text{(viii)}$$

Hence the validity condition becomes,

$$\frac{mZe^2}{\hbar^2k} |\ln(1-2ika)| < < 1$$

or
$$\frac{mZe^2}{\hbar^2 k} \sqrt{\{[\ln (1+4k^2a^2)^{1/2}]^2 + [\tan^{-1}(2ka)]^2\}} < < 1$$
 ...(ix)

{:
$$(1-2ika)=\sqrt{(1+a^2k^2)}e^{i\tan^{-1}(2ka)}$$
}

For low energy scattering, ka < < 1, and hence $\ln (1+4k^2a^2)^{1/2} \cong \ln 1=0$ and $\tan^{-1}(2ka) \cong 2ka$. Thus the validity condition (ix) simplifies to

$$\frac{2mZe^2a}{\hbar^2} < < 1 \qquad \dots(x)$$

From the Thomas-Fermi statistical theory, a is proportional to $Z^{-1/3}$ and hence the condition (x) is equivalent to $Z^{2/3} < < 1$; which is not true for any value of Z. Thus the Born-approximation can not be used for the scattering of low energy electrons by atoms.

For high energy electrons, ka > > 1. Therefore 1 can be neglected in the ln term compared to $4k^2a^2$ in Eqn. (ix). Also, $\tan^{-1}(2ka)$ cannot exceed $\pi/2$ and hence we can neglect it in comparison with the ln term. Thus the validity criteria becomes

$$\frac{mZe^2}{\hbar^2 k} \ln (2ka) < < 1$$

$$\frac{Ze^2}{\hbar v} \ln (2ka) < < 1, \qquad \dots (xi)$$

or

where $v = \frac{\hbar k}{m}$ is the velocity operator.

From (xi) we see that in the high energy limit, the Born-approximation is a good approximation for lighter elements only,

because $\frac{e^2}{\hbar v} > \frac{e^2}{\hbar c} \approx \frac{1}{137}$, as v cannot exceed the velocity of light c.

Thus the Born-approximation for the screened Coulomb potential is a good approximation for high incident energy and lighter atoms as scatterer.

Problem 6. Use the first Born-approximation to claculate the differential scattering cross-section for a potential such that $V=V_0$ for $0 \le r \le a$ and V=0 elsewhere.

Sol. The scattering amplitude in the first Born-approximation is given by

$$f(\theta) = -\frac{2m}{\hbar^2 K} \int_0^\infty r' \sin Kr \ V(r) \ dr$$

$$= -\frac{2mV_0}{h^2K} \int_0^a r \sin Kr \, dr$$

Evaluating the integral by parts, we obtain

$$f(\theta) = -\frac{2mV_0}{\hbar^2 K} \left[\frac{a \cos Ka}{K} - \frac{\sin Ka}{K^2} \right]$$

$$= \frac{2ma^3 V_0}{\hbar^2} \left(\frac{\sin Ka - Ka \cos Ka}{(Ka)^3} \right) \qquad \dots (i)$$

Hence the differential scattering cross section is given as $\left(\frac{d\sigma}{d\Omega}\right) = |f(\theta)|^2 = 4 \frac{m^2 a^6 V_0^2}{\hbar^2} \frac{(\sin Ka \quad Ka \cos Ka)^2}{(Ka)^6}$...(11)

Now, the condition for the validity of the Born-approxi-

mation becomes

$$\frac{m}{\hbar^{2}k} \left| \int_{0}^{\infty} (e^{2ikr} - 1) V(r) dr \right| < 1$$

$$\frac{mV_{0}}{\hbar^{2}k^{2}} \left| \int_{0}^{a} e^{2ik} - 1) k dr \right| < 1$$
...(iii)

or

Now, $\int_{0}^{a} (e^{2ikr} - 1) k dr = \left[\frac{e^{2ikr}}{2i} - kr\right]_{0}^{d}$ = $\frac{e^{2ika} - 1}{2i} - ka$

$$=e^{ika}\cdot\frac{e^{ika}-e^{-ika}}{2i}-ka$$

 $=(\cos ka+i\sin ka)\sin ka-ka$ $=(\cos ka \sin ka - ka) + i \sin^2 ka$

$$\left| \int_{0}^{a} (e^{2ikr} - 1) k dr \right| = \{ (\cos ka \sin ka - ka)^{2} + \sin^{4} ka \}^{1/2}$$

Hence the validity condition (iii) becomes

$$\frac{mV_0}{k^2\hbar^2} \{(\cos ka \sin ka - ka)^2 + \sin^4 ka\}^{1/2} < < 1 \qquad ...(iv)$$

If ka < < 1 (low energy limit) then we have $\sin ka \approx ka \text{ and } \cos ka \approx 1$...(v)

Hence from (iv) we have

$$\frac{mV_0}{k^2\hbar^2} \{ (1. ka - ka)^2 + (ka)^4 \}^{1/2} < < 1 \text{ or } \frac{mV_0a^2}{\hbar^2} < < 1 \dots \text{(vi)}$$

To satisfy (vi), V_0 and a should be very-very small. Thus the Born-appoximation in this case is valid for very-very weak potential of very small width.

For high energy (ka > > 1); sin ka and cos ka, which The The exceed unity, can be neglected in comparison with ka. The validity condition (iv) therefore, becomes

is.

$$\frac{mV_0a}{k\hbar^2} < < 1 \text{ or } \frac{V_0a}{v\hbar} < < 1 \qquad \dots \text{(vii)}$$

Thus the Born-approximation is a good approximation for high incident velocity v, and weak potential with small range.

Problem 7. Calulate the scattering cross-section in the first Born-approximation

(i) for the Gaussian potential

$$V(r) = V_0 \exp(-r^2/a^2)$$
 ...(i)

(ii) for the exponential potential

$$V(r) = V_0 \exp(-r/a)$$
 ...(ii)

(iii) and the potential

$$V(r) = V_0 r^2 \exp(-r^2/a^2)$$
 .. (iii)

In each case discuss the conditions for which the approximation is the best.

Sol. The scattering amplitude in the Born-approximation is written as

$$f(\theta) = -\frac{2m}{\hbar^2 K} \int_0^\infty r \sin Kr \ V(r) \ dr; \quad K = 2k \sin \theta/2 \qquad \dots \text{(iv)}$$

If the potential V(r) is an even function of r, it can be written as:

$$f(\theta) = -\frac{m}{\hbar^2 Ki} \int_{-\infty}^{+\infty} r e^{iKr} V(r) dr \qquad \dots (v)$$

The validity condition for Born-approximation has been seen to be

$$\frac{m}{\hbar^2 k} \left| \int_0^\infty \left(e^{2ikr} - 1 \right) V(r) dr \right| < < 1$$
 ...(vi)

For low energy, ka < < 1, where a is the range of the potential. Hence the first two terms in the series expansion of e^{2ikr} will be a very good approximation. Hence the condition (vi) for low energy case can be written as:

$$\frac{2m}{\hbar^2} \left| \int_0^\infty r \, V(r) \, dr \right| < < 1 \qquad \qquad \dots \text{(vii)}$$

If the kinetic energy of the particle is very large (ka > > 1), then the contribution of the oscillating term can be neglected and (vi) becomes

$$\frac{m}{\hbar^2 k} \left| \int_0^\infty V(r) \ dr \right| < < 1 \qquad \dots \text{(viii)}$$

(i) For the Gaussian potential, which is an even function of r, we write

$$f(\theta) = -\frac{mV_0}{\hbar^2 Ki} \int_{-\infty}^{+\infty} r e^{iKr} \cdot e^{-r^2/a^2} dr$$

$$= -\frac{mV_0}{\hbar^2 Ki} \int_{-\infty}^{+\infty} r \exp\left\{-\left(\frac{r}{a} - \frac{iKa}{2}\right)^2\right\} \cdot \exp\left\{-\frac{K^2 a^2}{4}\right\} dr$$
...(ix)

Putting,
$$t = \left(\frac{r}{a} - \frac{iKa}{2}\right); dt = \frac{dr}{a} \text{ or } dr = a dt; \text{ and } r = a\left(t + \frac{iKa}{2}\right),$$

we can write (ix) as:

can write (ix) as.
$$f(\theta) = -\frac{mV_0}{\hbar^2 K i} \cdot \exp. \left\{ -\frac{K^2 a^2}{4} \right\} \left[a^2 \int_{-\infty}^{+\infty} t e^{-t^2} dt + \frac{iKa^3}{2} \int_{-\infty}^{+\infty} e^{-t^2} dt \right]$$

The first integral on the right hand side of the above vanishes, because the integrand is an odd function of t. The value of the second integral is $\sqrt{(\pi)}$. Therefore,

$$f(\theta) = -\frac{mV_0 \exp \left\{-\frac{K^2 a^2/4}{\hbar^2 K i} \cdot \frac{iKa^3}{2} \sqrt{\pi}\right\}}{\frac{mV_0}{\hbar^2} \cdot \frac{a^3 \sqrt{\pi}}{2} \exp \left(-\frac{k^2 a^2 \sin^2 \theta}{2}\right) \dots (x)}$$

$$= -\frac{mV_0}{\hbar^2} \cdot \frac{a^3 \sqrt{\pi}}{2} \exp \left(-\frac{k^2 a^2 \sin^2 \theta}{2}\right) \dots (x)$$

The differential scattering cross-section is thus given by

$$\left(\frac{d\sigma}{d\Omega}\right) = |f(\theta)|^2 = \left(\frac{m!V_0}{\hbar^2}\right)^2 \frac{\pi a^3}{2} \cdot \exp\left(-2k^2a^2\sin^2\theta/2\right) \quad ...(xi)$$

The validity condition for low energy, eqn. (vii), can be written as:

$$\frac{2mV_0}{h^2} \left| \int_0^\infty r \, e^{-r^2/a^2} \, dr \right| < < 1$$

To evaluate the integral in the above, put $r^2/a^2 = z$.

$$\int_{0}^{\infty} r e^{-r^{2}/a^{2}} dr = \frac{a^{2}}{2} \int_{0}^{\infty} e^{-t} dt = \frac{a^{2}}{2} \left[-e^{-t} \right]_{0}^{\infty} = \frac{a^{2}}{2}$$

Therefore, the validity condition for low energy becomes

$$\frac{2mV_0a^2}{2\hbar^2} <<1 \qquad ...(xii)$$

To satisfy this condition, the strength of the potential 'Vo' should be very small. Thus the Born-approximation for low energy is a good approximation for very weak potential only.

For high energy, we have the validity condition (viii) as:

$$\frac{mV_0}{\hbar^2k} \left| \int_0^\infty e^{-r^2/a^2} dr \right| << 1$$

$$\frac{mV_0a\sqrt{(\pi)}}{2\hbar^2k} < < 1$$

...(xiii)

Thus the Born-approximation in this case is a very-very good approximation for high incident energy and weak potential.

(ii) In this case

$$f(\theta) = -\frac{2mV_0}{\hbar^2 K} \int_0^\infty r \sin K r \, e^{-r/a} \, dr$$

$$= -\frac{2mV_0}{\hbar^2 K} I_m \cdot \int_0^\infty r e^{iKr} \cdot e^{-r/a} \, dr$$

$$= -\frac{2mV_0}{\hbar^2 K} I_m \cdot \int_0^\infty \exp \left\{-r\left(\frac{1}{a} - iK\right)\right\} r \, dr \dots (xiv)$$

The integral in (xiv) can be evaluated by using,

$$\int_0^\infty e^{-\alpha x} x^n dx = \frac{n!}{\alpha^{n+1}}.$$

We get

$$f(\theta) = -\frac{2mV_0}{\hbar^2 K} I_m \cdot \frac{1}{(1/a - iK)^2} = -\frac{2mV_0}{\hbar^2 K} \cdot \frac{2Ka^3}{(1 + a^2K^2)^2}$$
$$= -\frac{4mV_0a^3}{\hbar^2 (1 + a^2K^2)^2} \dots (xv)$$

Hence the differential scattering cross-section is given by

$$\left(\frac{d\sigma}{d\Omega}\right) = |f(\theta)|^2 = \frac{16m^2V_0^2a^6}{\hbar^4(1+4k^2a^2\sin^2\theta/2)^2} \qquad ...(xvi)$$

In order to find the criteria for the validity of the Bornapproximation in this case, we have for the low incident energy, the validity condition as:

$$\frac{2mV_0}{\hbar^2} \left| \int_0^\infty re^{-r/a} dr \right| << 1$$

$$\frac{2mV_0a^2}{\hbar^2} << 1$$
...(xvii)

Oľ.

Similarly, for high incident energy, the condition for validity is given by

$$\frac{m}{\hbar^2 k} \left| \int_0^\infty V(r) \, dr \right| < < 1$$
or
$$\frac{mV_0}{\hbar^2 k} \left| \int_0^\infty e^{-r/a} \, dr \right| < < 1$$
or
$$\frac{mV_0 a}{\hbar^2 k} < < 1$$

...(xviii)

From (xvii) and (xviii) we see that the Born approximation 446 From approximation for the exponential potential if the inis a $\frac{good}{f}$ energy $(\hbar k)$ is high and the strength of $\frac{1}{2}$. is a good sight and the strength of the potential (V_0) cident energy ($\hbar k$) is high and the strength of the potential (V_0) cident so the approximation is valid for high. cident energy is small. So the approximation is valid for high incident energy potential. and weak potential.

(iii) In this case, the potential is an evenfunction of r,

therefore we write
$$f(\theta) = -\frac{m}{\hbar^2 K i} \int_{-\infty}^{+\infty} r e^{iKr} V(r) dr = -\frac{mV_0}{\hbar^2 K i} \int_{-\infty}^{+\infty} r^3 e^{iKr} e^{-r^2/a^2} dr$$

$$= -\frac{mV_0}{\hbar^2 K i} \cdot e^{-K^2 a^2/4} \int_{-\infty}^{+\infty} r^3 \exp \left\{ -\left(\frac{r}{a} - \frac{iKa}{2}\right)^2 \right\} dr$$
...(xix)

To evaluate the integral in (xix), we substitute

The first and the last integral in the right hand of the above equation vanishes, because the integrand is an odd function of t in both the cases. The second integral is a standard integral and it has the value $\sqrt{(\pi)}$. The third integral can be evaluated by using the formula

$$\int_{-\infty}^{+\infty} x^{2n} e^{-x^2} dx = \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)}{2^n} \sqrt{(\pi)},$$

and it has the value $\sqrt{(\pi)/2}$. Thus we have,

$$f(\theta) = -\frac{mV_0 a^5 \sqrt{(\pi)}}{8\hbar^2} (6 - K^2 a^2)$$

$$= -\frac{mV_0 a^5 \sqrt{(\pi)}}{4\hbar^2} \left(3 - 2k^2 a^2 \sin^2 \frac{\theta}{2}\right)$$

and

$$\left(\frac{d\sigma}{d\Omega} \right) = |f(\theta)|^2 = \frac{m^2 V_0^2 a^{10} \pi}{16\hbar^4} \left(3 - 2k^2 a^2 \sin^2 \frac{\theta}{2} \right)^2 \qquad ...(xx)$$

In order to find out the criteria for the validity of the Bornapproximation in this case, for low energy, we have the condition of validity as:

$$\frac{2mV_0}{\hbar^2} \left| \int_0^\infty r^3 e^{-r^2/a^2} dr \right| < < 1$$

The integral in it can be evaluated by the substitution $r^2/a^2=t$. We get:

$$\frac{2mV_0}{\hbar^2} \cdot \frac{a^4}{2} \left| \int_0^\infty t \, e^{-t} \, dt \right| << 1$$

$$\frac{2mV_0 a^4}{2\hbar^2} << 1 \qquad \dots (xxi)$$

or

7.

For high energy, validity condition is written as:

$$\frac{mV_0}{\hbar^2 k} \left| \int_0^\infty r^2 e^{-r^2/a^2} dr \right| << 1$$
or
$$\frac{mV_0 a^3}{\hbar^2 k} \left| \int_0^\infty \frac{r^2}{a^2} \cdot e^{-r^2/a^2} d\left(\frac{r}{a}\right) \right| << 1$$
or
$$\frac{mV_0 a^3 \sqrt{(\pi)}}{4\hbar^2 k} << 1 \qquad ...(xxii)$$

From the validity conditions (xxi) and (xxii) we see that the Born-approximation is a good approximation for weak potential and high incident energy.

Problem 8. A high energy electron collides with a hydrogen atom in its ground state and excites it to the 2p-states. Calculate the scattering cross-section for this process by using the Bornapproximation for electron-atom scattering.

Sol. In the Born-approximation, the scattering amplitude for the process in which the atom in the initial state w_a is excited to the state w_b is given by Eqn. (190)

$$f(a \to b) = -\frac{2me^2}{\hbar^2 K^2} \int e^{i\mathbf{K} \cdot \mathbf{r}} w_b^*(r) w_a(r) d^3r \qquad ...(i)$$

In the present case, the initial state w_a is the ground state of the hydrogen atom and the state w_b is the 2p-states of hydrogen. Therefore

$$w_a(r) = \psi_{100} = \frac{1}{\sqrt{(\pi a_0^3)}} e^{-r/a_0},$$
and
$$w_b(r) = \psi_{21m} = \frac{1}{2\sqrt{(6)}} \frac{1}{\sqrt{(a_0^3)}} \cdot \frac{r}{a_0} \cdot e^{-r/2a_0} Y_1^m(\theta, \phi)$$

Using these into (i) we get the scattering amplitude as

$$f(1s \to 2p) = -\frac{2}{a_0 K^2} \cdot \frac{1}{\sqrt{(6)a_0^3}} \cdot \frac{1}{\sqrt{(4\pi)}} \cdot \frac{1}{a_0} \int e^{i\mathbf{K} \cdot \mathbf{r}} r$$

$$\times \exp \left\{ -\frac{3r}{2a_0} \right\} Y_i^m (\theta, \phi) d^3r \left\{ :: a_0 = \frac{\hbar^2}{me^2} \right\}$$

Now, the plane wave $e^{i\mathbf{K}\cdot\mathbf{r}}$ can be expressed in terms of the Bessel's function and the spherical harmonics as:

$$e^{i\mathbf{K}.\mathbf{r}} = \sum_{l=0}^{\infty} 4\pi i^{l} j_{l} (Kr) \sum_{m'=-l}^{+l} Y_{l}^{m'*} (\theta_{k}, \phi_{k}) Y_{l}^{m'} (\theta, \phi) ...(ii)$$

$$\therefore \int e^{i\mathbf{K}.\mathbf{r}} Y_{1}^{m} (\theta, \phi) d\Omega = \sum_{l, m'} 4\pi i^{l} j_{l} (Kr) Y_{l}^{m'*} (\theta_{K}, \phi_{K})$$

$$\times \int Y_{l}^{m'} Y_{1}^{m} d\Omega$$

$$= \sum_{l, m'} 4\pi i^{l} j_{l} (Kr) Y_{l}^{m'*} (\theta_{K}, \phi_{K}) \delta_{l1} \delta_{mm'}$$

$$= 4\pi i j_{1} (Kr) Y_{1}^{m*} (\theta_{K}, \phi_{K}) ...(iii)$$

Using it we have,

$$f(1s \to 2p) = -\frac{2}{K^2 a_0^5 \sqrt{(24\pi)}} \cdot \int_0^\infty 4\pi i \, j_1(Kr) \, Y_1^{m^*}(\theta_K, \phi_K) \times e^{-3r/2a_0} \, r^3 \, dr \qquad \dots \text{(iv)}$$

The integral in (iv) can be evaluated as follows:

$$\int_{0}^{\infty} r^{8}e^{-3r/2a_{0}} j_{1}(Kr) dr = \int_{0}^{\infty} r^{3} e^{-3r/2a_{0}} \left\{ \frac{\sin Kr}{(Kr)^{2}} - \frac{\cos Kr}{Kr} \right\} dr$$

$$= \frac{1}{K^{2}} \int_{0}^{\infty} r e^{-3r/2a_{0}} \sin Kr dr - \frac{1}{K} \int_{0}^{\infty} r^{2} e^{-3r/2a_{0}} \cos Kr dr$$

$$= \frac{1}{K^{2}} I_{m} \cdot \int_{0}^{\infty} r e^{-3r/2a_{0}} \cdot e^{iKr} dr$$

$$- \frac{1}{K} \operatorname{Rel.} \int_{0}^{\infty} r^{2} e^{-3r/2a_{0}} \cdot e^{iKr} dr$$

$$= \frac{1}{K^{2}} I_{m} \cdot \frac{1}{\left(\frac{3}{2a_{0}} - iK\right)^{2}} - \frac{1}{K} \operatorname{Rel.} \cdot \frac{2}{\left(\frac{3}{2a_{0}} - iK\right)^{3}}$$

$$= \frac{1}{K^{2}} \cdot \frac{\frac{3K}{a_{0}}}{\left(\frac{9}{4a_{0}^{2}} + K^{2}\right)^{2}} - \frac{2}{K} \cdot \frac{\frac{27}{8a_{0}^{3}} - \frac{9K^{2}}{2a_{0}}}{\left(\frac{9}{4a_{0}^{2}} + K^{2}\right)^{3}}$$

$$= \frac{12Ka_{0}^{5}}{\left(\frac{9}{4} + K^{2}a_{0}^{2}\right)^{3}} \cdot ..(v)$$

$$f(1s \longrightarrow 2p) = -\frac{96i\sqrt{(\pi)}}{\sqrt{(24)}} \cdot Y_1^{m^*} (\theta_K, \phi_K) \cdot \frac{1}{\left(\frac{9}{4} + K^2 a_{0^*}\right)^3} \cdot \text{Sels}$$
...(vi)

Hence the differential scattering cross-section is given by:

Experimentally, we cannot resolve the different values of m and hence we measure the cross-section

Therefore we have
$$\sigma_{1s \to 2p} = \sum_{m=-1}^{+1} \left(\frac{d\sigma}{d\Omega} \right) = \frac{384\pi}{K^2} \cdot \frac{k_{2p}}{k_{1s}} \cdot \sum_{m=-1}^{+1} Y_1^{m^*} \quad Y_1^m \cdot \frac{1}{\left(\frac{9}{4} + K^2 a_0^2 \right)} \cdot \frac{1}{\left($$

The quantum mechanics based on the Schroedinger equation can describe the particles with velocity much lesser than that of light, i.e., it can describe only non-relativistic particles. Morelight, i.e., Schroedinger's theory fails to explain the spin of a over, the Schroedinger's theory fails to explain the spin of a particle and it cannot give a satisfactory account of high energy phenomena like pair production, bremsstrahlung and zetterbewegung etc. In this chapter we shall formulate a theory which can describe the motion of a particle that has a speed approaching that of light. We shall also show that this theory automatically incorporates the phenomena which had to be added afterwards in the non-relativistic theory. For the development of the relativistic theory we are guided by the following points:

- (i) The theory should be formulated in terms of an amplitude function to which we can assign the customary statistical interpretation, as in the case of Schroedinger wave-function.
- (ii) The description of physical phenomena in the theory should be based on an equation of motion describing the development of the system in time.
- (iii) The superposition principle should hold and therefore, equation of motion must be linear in the amplitude function.
- (iv) The equation of motion must be invariant under Lorentz transformations.
- (v) The theory should be consistent with the correspondence principle, and in the non-relativistic limit it should reduce to the standard form of quantum mechanics for non-relativistic particles.

The basic equation for a free particle in non-relativistic case is the Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t}, \qquad \dots (1)$$

where $\frac{-\hbar^2}{2m} \nabla^2 = H$, is the Hamiltonian operator for the free particle. In order to write an equation of motion for a relativistic free particle, we should start with the relativistic Hamiltonian, H,

$$H^2 = p^2c^2 + m^2c^4,$$
 ...(2)

Here, p is the linear momentum of the particle, c the velocity of light and m is the rest mass of the particle. From (2) we have

$$H = \pm c\sqrt{(p^{2} + m^{2}c^{2})}$$

$$= \pm c\sqrt{\left\{-\hbar^{2}\left(\frac{\partial^{2}}{\partial x^{2}} + \frac{\partial^{2}}{\partial y^{2}} + \frac{\partial^{2}}{\partial z^{2}}\right) + m^{2}c^{2}\right\}} \qquad ...(3)$$

$$\left\{ : p_{x} = -i\hbar \frac{\partial}{\partial x}; p_{y} = -i\hbar \frac{\partial}{\partial y} \text{ and } p_{z} = -i\hbar \frac{\partial}{\partial z} \right\}.$$

Upper sign in (3) gives positive energy and lower sign yields negative value of the energy. In classical relativity, the second alternative is of no physical significance and can be disregarded. Therefore,

$$H = +c \sqrt{\left\{-\hbar^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + m^2 c^2\right\}}. \qquad ...(4)$$

This operator is rather complicated. If it would be used in Schroedinger equation $H\psi = E\psi$, it would no longer be a differential equation of finite order. The fundamental difficulty, however, is that adopting this operator makes it impossible to construct expressions for probability current and probability density, which satisfy a relativistic equation for the conservation of probability. Moreover, the equation won't be invariant under Lorentz transformation, because it is of second order in space while it is of first order in time. Clearly, some modification is needed.

10.1. THE KLEIN-GORDAN EQUATION:

To avoid the difficulties of the Schroedinger's relativistic wave equation, discussed above, Klein and Gordan developed an equation by operating (2) on a wave function $\phi(\mathbf{r}, t)$. The result is $(p^2c^2+m^2c^4)\phi(\mathbf{r}, t)=E^2\phi(\mathbf{r}, t)$.

Replacing p and E, in (5), by the differential operators $-i\hbar\nabla$ and $i\hbar\frac{\partial}{\partial t}$; respectively, we get

$$-\hbar^2 c^2 \nabla^2 \phi(\mathbf{r}, t) + m^2 c^4 \phi(\mathbf{r}, t) = -\hbar^2 \frac{\partial^2 \phi(\mathbf{r}, t)}{\partial t^2}$$
Equation (6) has a 1

Equation (6) has a plane wave solution of the form

$$\phi(\mathbf{r}, t) = e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} \dots (7)$$

which are the eigenfunctions of the operators E and p with eigenvalues $\hbar \omega$ and $\hbar k$; respectively. It is apparant that (7) satisfies (6) if

 $\hbar \omega = \pm (\hbar^2 c^2 k^2 + m^2 c^4)^{1/2}.$ (8)

The positive and negative square-roots in (8) correspond to an ambiguity in the sign of the energy that also results from the classical expression (2).

Equation (6) can also be written as:

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \phi(\mathbf{r}, t) = \frac{m^2 c^2}{\hbar^2} \phi(\mathbf{r}, t)$$
or
$$\left(\Box - \frac{m^2 c^2}{\hbar^2}\right) \phi(\mathbf{r}, t) = 0, \qquad \dots (9)$$

where, $\Box = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}$ is known as d' Alembertian operator.

Equation (9) is the famous Klein-Gordan equation of motion. This equation can describe only spinless particles such as π -mesons. Particles with finite spin value cannot be discussed with this equation.

Charge and current Densities. In order to find the expressions for charge and current densities and to derive the equation of continuity, we start with the Klein-Gordan (K. G.) equation

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2}\right) \phi(\mathbf{r}, t) = 0. \tag{10}$$

Taking its complex conjugate,

$$\left(\nabla^{2} - \frac{1}{c^{2}} \frac{\partial^{2}}{\partial t^{2}} - \frac{m^{2}c^{2}}{\hbar^{2}}\right) \phi^{*} (\mathbf{r}, t) = 0. \tag{11}$$

Multiplying from left, equation (10) by ϕ^* and (11) by ϕ and then subtracting one from the other, we get

$$\frac{\hbar}{2im} \left(\phi^* \nabla^2 \phi + \phi \nabla^2 \phi^* \right) + \frac{i\hbar}{2mc^2} \left(\phi^* \frac{\partial^2 \phi}{\partial t^2} - \phi \frac{\partial^2 \phi^*}{\partial t^2} \right) = 0$$

$$\frac{\partial P(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{S}(\mathbf{r}, t) = 0, \qquad \dots (12)$$

or where

$$P(\mathbf{r}, t) = \frac{i\hbar}{2mc^2} \left(\phi^* \frac{\partial \phi}{\partial t} - \phi \frac{\partial \phi^*}{\partial t} \right),$$

$$S(\mathbf{r}, t) = \frac{\hbar}{2im} \left(\phi^* \nabla \phi - \phi \nabla \phi^* \right).$$
(13)

and

Equation (12) is identical to the non-relativistic probability conservation equation. Expression for the current S is the same

as in the non-relativistic case, but the probability $P(\mathbf{r}, t)$ is not necessarily positive, so that it can be interpreted as the position probability density. To see it, we have the following two solutions of the K.G. equation;

and
$$\phi^{(+)}(\mathbf{r}, t) = \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega_{+} t)],$$

 $\phi^{(-)}(\mathbf{r}, t) = \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega_{-} t)],$...(14)

corresponding to positive and the negative values of the energy; respectively. ω_+ and ω_- are the values of ω from (8) with positive and the negative signs; respectively. $\phi^{(+)}(\mathbf{r}, t)$ gives a positive probability while $\phi^{(-)}(\mathbf{r}, t)$ gives the negative probability. We may arbitrarily omit all solutions $\phi^{(-)}(\mathbf{r}, t)$ with negative energy to make the probability positive. But it is unjustified because the solutions $\phi^{(+)}(\mathbf{r}, t)$ with positive energy alone do not form a complete set. Pauli and Weisskopf proposed that $P(\mathbf{r}, t)$ multiplied by the charge of the particle can be interpreted as charge density which can be positive as well as negative so long as it is real.

It can be shown that in agreement with the correspondence principle, in the non-relativistic limit, P(r, t) reduces to the usual expression $\phi^*(r, t) \phi(r, t)$. For it, using the stationary state (7) into (13), we get

$$P(\mathbf{r}, t) = \frac{\hbar \omega}{mc^2} \phi^*(\mathbf{r}, t) \phi(\mathbf{r}, t).$$
 ...(15)

In the non-relativistic limit, |p| << mc. Therefore, it can be seen from (8) that $\hbar\omega \approx mc^2$, and that (15) becomes the well known non-relativistic expression for the probability density

$$P(\mathbf{r},t)\approx \phi^*(\mathbf{r},t) \phi(\mathbf{r},t) = |\phi(\mathbf{r},t)|^2$$
...(16)

10.2. K. G. EQUATION FOR A CHARGED PARTICLE IN AN E. M. POTENTIAL:

If -e is the charge of the particle (electron), and if the e.m. potential is characterized by the scalar potential ϕ and the vector potential $A(\mathbf{r}, t)$, then the effect of the e.m. field on the particle

can be introduced by replacing p by $p - \frac{e}{c}$ A and E by $E - e \varphi$.

Thus the relativistic energy momentum relation becomes

$$(E-ep)^{2} = \left(p - \frac{e}{c}A\right)^{2}c^{2} + m^{2}c^{4} \qquad ...(17)$$

$$(E-ep)^{2} = (cp-eA)^{2} + m^{2}c^{4}.$$

or

Operating (17) on the function ϕ (r, t), after replacing E and p by the differential operators in $\frac{\partial}{\partial t}$ and $--i\hbar \nabla$, we get the K.G. equation for a charged particle in an e.m. potential as:

$$\left(i\hbar \frac{\partial}{\partial t} - e\varphi\right)^{2} \phi(\mathbf{r}, t) = (-i\hbar c \nabla - eA)^{2} \phi(\mathbf{r}, t) + m^{2}c^{4} \phi(\mathbf{r}, t).$$
(18)

Now, the L.H.S. of (18) can be written as

$$\begin{split} \left(i\hbar\frac{\partial}{\partial t}-e\varphi\right)\left(i\hbar\frac{\partial\phi}{\partial t}-e\varphi\phi\right) \\ &=\left(-\hbar^2\frac{\partial^2\phi}{\partial t^2}-i\hbar e\frac{\partial}{\partial t}\frac{(\varphi\phi)}{\partial t}-i\hbar e\varphi\frac{\partial\phi}{\partial t}+e^2\varphi^2\phi'\right) \\ &=\left(-\hbar^2\frac{\partial^2\phi}{\partial t^2}-2i\hbar e\varphi\frac{\partial\phi}{\partial t}-i\hbar e\phi\frac{\partial\varphi}{\partial t}+e^2\varphi^2\phi'\right), \end{split}$$

and the R.H.S. is

 $(--\hbar^2c^2\nabla^2+2i\hbar ce\ A\cdot\nabla+i\hbar ce\ \nabla\cdot A+e^2A^2+m^2c^4)\ \phi.$ Therefore, (18) can be written as:

$$\left(-\hbar^{2}\frac{\partial^{2}}{\partial t^{2}}-2ie\hbar\varphi\frac{\partial}{\partial t}-i\hbar e\dot{\varphi}\frac{\partial\varphi}{\partial t}+e^{2}\varphi^{2}\right)\dot{\varphi}\left(\mathbf{r},t\right)$$

$$=\left(-\hbar^{2}c^{2}\nabla^{2}+2i\hbar ce\mathbf{A}\cdot\nabla+i\hbar ce\nabla\cdot\mathbf{A}+e^{2}A^{2}+m^{2}c^{4}\right)\dot{\varphi}\left(\mathbf{r},t\right).$$

$$=\left(-\hbar^{2}c^{2}\nabla^{2}+2i\hbar ce\mathbf{A}\cdot\nabla+i\hbar ce\nabla\cdot\mathbf{A}+e^{2}A^{2}+m^{2}c^{4}\right)\dot{\varphi}\left(\mathbf{r},t\right).$$
(19)

To check the correctness of equation (19), let us take its nonrelativistic limit. We make the substitution ...(20).

nit. We make the substitute
$$\phi$$
 (r, t) = ψ (r, t) exp. $\{-imc^2t/\hbar\}$, ...(20)

where mc^2 is the rest mass energy of the particle. Then

is the rest mass energy of
$$\frac{\partial \phi}{\partial t} = \left(\frac{\partial \psi}{\partial t} - \frac{imc^2}{\hbar}\psi\right) \exp\left\{-imc^2t/\hbar\right\}, \text{ and}$$

$$\frac{\partial^2 \phi}{\partial t^2} = \left(\frac{\partial^2 \psi}{\partial t^2} - \frac{2imc^2}{\hbar}\frac{\partial \psi}{\partial t} - \frac{m^2c^4}{\hbar^2}\psi\right) \exp\left\{-imc^2t/\hbar\right\}.$$
...(21)

Assuming that the operation of $i\hbar \frac{\partial}{\partial t}$ on ψ gives a result of the order of $e\varphi\psi$ which is small in comparison with $mc^*\psi$, the first term in both of the above derivatives can be neglected, as can the last two terms on the left hand side of (19) which then becomes:

...(28)

It is clearly the non-relativistic electromagnetic Schroedinger equation.

10.3. SOLUTION OF K. G. EQUATION WITH COULOMB POTENTIAL:

Equation (19) can be separated w.r.t. r and t if the potentials A, φ are time independent. We then write

$$\phi(\mathbf{r}, t) = u(\mathbf{r}) \exp[-iEt/\hbar]$$
 ...(23)

Substituting it into (19) we get,

$$(E - e\varphi)^2 u(\mathbf{r}) = (-\hbar^2 c^2 \nabla^2 + 2i\hbar ce \mathbf{A} \cdot \nabla + i\hbar ce \nabla \cdot \mathbf{A} + e^2 A^2 + m^2 c^4) u(\mathbf{r}) \qquad \dots (24)$$

We now specialize to the case in which A=0 and φ is spherically symmetric. Equation (24) then becomes

$$(E - e\varphi)^2 u(\mathbf{r}) = (-\hbar^2 c^2 \nabla^2 + m^2 c^4) u(\mathbf{r}) \qquad ...(25)$$

Equation (25) can be used to describe the problem of hydrogen atom, because in case of hydrogen atom A=0, since there is no magnetic field,

and

U

$$V(r) = e\varphi = -\frac{ze^2}{r}$$
 is a central potential.

Using it in (25) we get

$$\left(E + \frac{ze^{2}}{r^{2}}\right)^{2} u(\mathbf{r}) = \left(-\hbar^{2}c^{2} \nabla^{2} + m^{2}c^{4}\right) u(\mathbf{r})$$

$$\left[-\frac{1}{r^{2}} \frac{d}{dr} \left(r^{2} \frac{d}{dr}\right) + \frac{L^{2}}{\hbar^{2}r^{2}}\right] u(\mathbf{r}) = \frac{\left(E + \frac{ze^{2}}{r}\right) - m^{2}c^{4}}{\hbar^{2}c^{2}} u(\mathbf{r})$$

$$\left\{ \because \nabla^{2} = \frac{1}{r^{2}} \frac{d}{dr} \left(r^{2} \frac{d}{dr}\right) - \frac{L^{2}}{\hbar^{2}r^{2}} \right\}$$
...(26)

We can separate the radial and the angular parts by substitu-

$$u(\mathbf{r}) = R_l(r) Y_l^m(\theta, \phi) \qquad ...(27)$$

into equation (26) we have

$$\left[-\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{l (l+1)}{r^2} \right] R_l(r) = \frac{\left(E + \frac{ze^3}{r} \right)^2 - m^2 c^4}{\hbar^2 c^2} R_l(r)$$
Decause $L^2 Y_l^m = \hbar^2 l (l+1)$; $l = 0, 1, 2, ...$

Or $\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR_l}{dr} \right) + \frac{E^2 - m^2 c^4}{\hbar^2 c^2} R_l + \frac{2Eze^2}{\hbar c^2} \frac{R_l}{r}$

$$\frac{l (l+1) - r^2 c^4 l \hbar^2 c^2}{r^2}$$

Putting $\rho = \alpha r$, eqn. (28) can be written as:

$$\frac{1}{\rho^{2}} \frac{d}{d\rho} \left(\rho^{2} \frac{dR_{I}}{d\rho} \right) + \frac{E^{2} - m^{2}c^{4}}{\alpha^{2}\hbar^{2}c^{2}} R_{I} + \frac{2Eze^{2}}{\hbar^{2}c^{2}\alpha} \cdot \frac{R_{I}}{\rho} \\
- \frac{l(l+1) - z^{2}e^{4}/\hbar^{2}c^{2}}{\rho^{2}} R_{I} = 0$$
or
$$\frac{1}{\rho^{2}} \frac{d}{d\rho} \left(\rho^{2} \frac{dR_{I}}{d\rho} \right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1) - \gamma^{2}}{\rho^{2}} \right] R_{I} = 0$$
where,

$$\alpha^{2} = \frac{4 \left(m^{2}c^{4} - E^{2}\right)}{\hbar^{2}c^{2}}$$

$$\gamma = ze^{2}/\hbar c, \text{ and}$$

$$\lambda = \frac{2E\gamma}{\hbar c\alpha}$$

$$(30)$$

To solve eqn. (29), we see that the solution of the asymptotiform $(\rho \rightarrow \infty)$ of it,

$$\frac{d^2R_1}{d\rho^2} - \frac{1}{4} R_1 = 0 \qquad ...(31)$$

is given by $R_i = \exp[\pm \rho/2]$. The boundary condition that the solution should vanish in the asymptotic region, permits us to keep only the negative sign in the exponent. This suggests that it might be possible to find an exact solution of (29) of the form

$$R_{I}(\rho) = F(\rho) \exp[-\frac{1}{2}\rho]$$
 ...(32)

where F(P) is a polynomial of finite degree in P.

$$\frac{dR_{i}(\rho)}{d\rho} = \{F'(\rho) - \frac{1}{2} F(\rho)\} \exp \left[-\frac{1}{2}\rho\right], \qquad ...(33)$$

and

$$\frac{d^2R_l(\rho)}{d\rho^2} = \{F''(\rho) - F'(\rho) + \frac{1}{4}F(\rho)\} \text{ exp. } [-\frac{1}{2}\rho] \dots (34)$$

Using eqns. (32) through (34) in to (29), we get

$$F''(\rho) + \left(\frac{2}{\rho} - 1\right)F'(\rho) + \left(\frac{\lambda - 1}{\rho} - \frac{l(l+1) - \gamma^2}{\rho^2}\right)F(\rho) = 0$$

or

$$\begin{array}{ll}
\rho^2 F'' + (2\rho - \rho^2) F'' + [(\lambda - 1) \rho - \{l(l+1) - \gamma^2\}] F = 0 \dots (35) \\
\text{n. be solved for } F \text{ by the points}
\end{array}$$

It can be solved for F by the method of power series:

$$F(\rho) = \sum_{n} C_n \rho^{s \neq n} ; C_0 \neq 0 \qquad ... (36)$$

where s is so chosen that the solution is well defined at the origin.

Substituting (36) into (35) and equating the coefficients of the coefficients C_k 's

$$(s+k+1) (s+k) C_{k+1} + 2(s+k+1) C_{k+1} - (s+k) C_k + (\lambda-1) C_{k} - l(l+1) C_{k+1} + \gamma^2 C_{k+1} = 0 \qquad ...(37)$$

Similarly, equating the coefficients of ps equal to zero we get:

or $s(s-1) C_0 + 2s C_0 - l(l+1) C_0 + \gamma^2 C_0 = 0$ $s(s+1) - l(l+1) + \gamma^2 = 0 \qquad ...(38)$

For the solution to well defined at be the origin we should hence $s \ge 0$. Then, for the regular solution of (35) the coefficients of successive terms in series of eqn. (36) should satisfy (37), from which we can write

$$C_{k+1} = \frac{s+k+1-\lambda}{(k+1)(2s+k+2)} C_k \qquad \dots (39)$$

The series governed by (39) does not lead to a satisfactory solution unless the series breaks off after a finite number of terms. The series breaks off after the nth term if we set $C_{n'+2}=0$. Then from (39):

 $n'+s+1-\lambda=0$ or $\lambda=n'+s+1$...(40)

Clearly, n' must be zero or a positive integer. Now,

$$\lambda^{2} = \frac{2E\gamma}{\hbar c\alpha}$$

$$\therefore \lambda = \frac{4E^{2}\gamma^{2}}{\hbar^{2}c^{2}\alpha^{2}} = \frac{E}{m^{2}c^{4} - E^{2}} \Rightarrow$$

$$E = mc^{2} \left(1 + \gamma^{2}/\lambda^{2}\right)^{-1/2} \qquad \dots (41)$$

This gives the energy for the hydrogen atom, where λ is given by (40) and s is the solution of eqn. (38). Equation (38) has two roots given by

 $s = -\frac{1}{2} \pm \frac{1}{2} \left[(2l+1)^2 - 4\gamma^2 \right]^{1/2}, \qquad ...(42)$

out of which one is positive and the other one is negative for all l>0, For l=0 both are negative, but γ is very small (very nearly equal to z/137) so that the use of the upper sign in (42) gives a value of s that is close to zero for physically interesting values of z. Thus $R_l(r)$, which behaves like r^s near r=0, is though singular, the singularity is mild. The charge density $eP(\mathbf{r}, t)$ is still well defined at the origin. We thus use the upper sign in (42) for all values of l and obtain from (40):

$$\lambda = n' + \frac{1}{2} + \frac{1}{2} \left[(2l+1)^2 - 4\gamma^2 \right]^{1/2}$$

$$= n' + \frac{1}{2} + \left(l + \frac{1}{2} \right) \left[1 - \frac{\gamma^2}{(l + \frac{1}{2})^2} \right]^{2\gamma_1}$$

$$= n' + \frac{1}{2} + \left(l + \frac{1}{2} \right) \left[1 - \frac{\gamma^2}{2(l + \frac{1}{2})^2} - \frac{1}{8} - \frac{\gamma^4}{(l + \frac{1}{2})^4} + \dots \right]$$

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$$= n' + \frac{1}{2} + \left(l + \frac{1}{2}\right) - \frac{1}{2} \frac{\gamma^2}{(l + \frac{1}{2})} - \frac{1}{8} \frac{\gamma^4}{(l + \frac{1}{2})^3} + \dots$$

$$\cong (n' + l + 1) - \frac{1}{2} \frac{\gamma^2}{(l + \frac{1}{2})} - \frac{1}{8} \frac{\gamma^4}{(l + \frac{1}{2})^3}$$
or $\lambda \cong n - \frac{1}{2} \frac{\gamma^2}{l + \frac{1}{2}} - \frac{1}{8} \frac{\gamma^4}{(l + \frac{1}{2})^3}$
where $n = (n' + l + 1)$ is the standard of the sta

where n = (n'+l+1) is the total quntum number and it takes

Using (43), the energy levels (41) are given by:

$$E = mc^{2} \left[1 - \frac{1}{2} \frac{\gamma^{2}}{\left(n - \frac{\gamma^{2}}{2l + 1}\right)^{2}} + \frac{3}{8} \frac{\gamma^{4}}{\left(n - \frac{\gamma^{2}}{2l + 1}\right)^{4}} \right]$$

$$= mc^{2} \left[1 - \frac{\gamma^{2}}{2n^{2}} - \frac{\gamma^{2}}{2n^{2}} \cdot \frac{1}{n} \cdot \frac{2\gamma^{2}}{(2l + 1)} + \frac{3\gamma^{4}}{8n^{4}} \right]$$
or $E = mc^{2} \left[1 - \frac{\gamma^{2}}{2n^{2}} - \frac{\gamma^{4}}{2n^{4}} \left(\frac{n}{l + \frac{1}{2}} - \frac{3}{4} \right) \right]$
The first term and the second seco

The first term on the r.h.s. of (44) is the rest mass energy; the second term

$$-\frac{mc^2}{2n^2} \frac{\gamma^2}{2n^2} = -\frac{mz^2}{2n^2} \frac{e^4}{\hbar^2}$$

is the non-relativistic Rydberg's term. The third term removes the degeneracy of states with the same n but different l; this is the fine structure energy. The fine structure obtained here does not agree with experimentally observed fine structure of the hydro-

10.4. DIFFICULTIES OF K. G. EQUATION AND DEVELOP-MENT OF DIRAC EQUATION:

Although the Klein Gordon equation is quite satisfactory when properly interpreted, there are many difficulties in describing an electron with it. It describes only spinless particles and cannot accommodate the spin of the electron. Further, the probability density for the K.G. particle is not positive definite Further more, K.G equation does not give the experimentally observed fine structure of the hydrogen atom; and it is not able to associate any physical significance to the negative energy states.

From the derivation of the equation of continuity for K.G. equation, it is clear that the appearance of the linear time derivative is unavoidable in the expression for $P(\mathbf{r}, t)$, so long as the wave function satisfies a partial differential equation which is

quadratic in the time derivative. We can avoid this difficulty, and hence the difficulty of negative $P(\mathbf{r}, t)$ by developing a relativistic wave equation which is linear in the time derivative. This was done by Dirac in 1928, who derived an equation linear in the time derivative which is relativistically invariant and gives positive definite probability It describes the particle with spin ½ and there exists very good physical interpretation of the negative energy solutions of this equation? We now follow the historic path taken by Dirac to develop this equation.

The energy E of a classical relativistic particle is given by

the relation:

$$E^{2} = p^{2}c^{2} + m^{2}c^{4}$$
 ...(45)

The classical relativistic Hamiltonian for a free particle is the positive square root of the right hand side of (45). Keplacing p $cy-i\hbar$ ∇ in this Hamiltonian, we get a wave equation unsymmetrical with respect to space and time derivatives. Dirac modified this Hamiltonian in such a way as to make it linear in the space derivative. In order to linearize the Hamiltonian in momentum and in mass terms, we must express the quantity,

$$p^{2}c^{2} + m^{2}c^{4} = c^{2} (f_{x}^{2} - p_{y}^{2} + p_{z}^{2}) + m^{2}c^{4} \qquad ... (46)$$

as a perfect square. The simplest possibility is like,

as a perfect square. The stapped
$$p_x^2 + p_y^2 + p_z^2 + m^2c^2 = (\alpha_x p_x + c_y p_y + \alpha_z p_z + \beta mc)^2$$
. ...(47)
 $p_x^2 + p_y^2 + p_z^2 + m^2c^2 = (\alpha_x p_x + c_y p_y + \alpha_z p_z + \beta mc)^2$(47)
where the coefficients α_x , α_y , α_z and β are yet to be determined.
We cannot satisfy (47) by taking α 's and β to be ordinary num-

bers. In fact we have $(\alpha_z p_x + \alpha_y p_y + \alpha_z \dot{p}_z + \varepsilon_m c)^2 = \alpha_x^2 p_x^2 + \alpha_x \alpha_y p_x p_y + \alpha_x \alpha_z p_x p_z +$ $\alpha_x\beta p_x mc + \alpha_y x_x p_y p_x + \alpha_y^2 p_y^2 + \gamma_y \alpha_z p_y p_z + \alpha_y \beta p_y mc + \alpha_z \alpha_x p_z p_x +$ $\alpha_z \circ_y p_z p_y + \alpha_z^2 p_z^2 + \alpha_z \xi p_z mc + \beta \alpha_x p_x mc + \beta \alpha_y p_y mc + \xi \alpha_z p_z mc + \alpha_z p_z mc + \beta \alpha_$

 $\beta^2 ni^2 c^2$.

If $\alpha's$ and β are ordinary numbers, then the right hand side of (47) involves the cross products of p's which do not appear on the left hand side. But if we take α 's and β as operators with the commutation relations,

$$\alpha_{x}\alpha_{y} = -\alpha_{y}\alpha_{z}; \alpha_{x}\alpha_{z} = -\alpha_{z}\alpha_{x}; \alpha_{y}\alpha_{z} = -\alpha_{z}\alpha_{y}; \alpha_{x}\beta = -\beta\alpha_{x};$$

$$\alpha_{y}\beta = -\beta\alpha_{y}; \alpha_{z}\beta = -\beta\alpha_{z},$$

$$(48)$$

then the cross products cancel out, because p's commute with one another, and hence the right hand side of (47) becomes:

$$\sigma_x^2 p_x^2 + \sigma_y^2 p_y^2 + \sigma_z^2 p_z^2 + \xi^2 m^2 c^2 \qquad \dots (49)$$

If we further take

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$$
 ...(50)

then (47) is satisfied in every detail.

Thus we conclude that if α 's and β are operators satisfying (48) and (50), then the square-root of (46) can be written as:

 $\pm c(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta mc) \qquad ...(51)$

Replacement of α 's by $-\alpha$'s and β by $-\beta$ do not alter (48) and therefore (50), it is immaterial whether we take the upper or the lower sign in (51). Taking the positive sign \dagger in (51) we write the Dirac Hamiltonian as:

$$H = c(\alpha_{x}p_{x} + \alpha_{y}p_{y} + \alpha_{z}p_{z}) + \beta mc^{2}$$

$$= cx \cdot \mathbf{p} + \beta mc^{2}$$

$$= -i \operatorname{fic} \alpha \cdot \nabla + \beta mc^{2} \qquad ...(52)$$

Using (52) we get the Dirac's relativistic wave equation $H\psi = E\phi$ as:

$$i\hbar \frac{\partial \psi}{\partial t} = (-i\hbar c \, \vec{\alpha} \, \cdot \, \nabla + \beta mc^2)\psi \qquad ...(53)$$

To characterize equation (53) completely, we need to find the matrices α 's and β , called the *Dirac matrices*. For a simple representation of these matrices, we shall make use of the properties these matrices should satisfy:

First of all α_x , α_y , α_z and β should be hermitian in order that the Hamiltonian H be a Hermitian operator.

From (50) we see that the eigenvalues of all of these four matrices should be ± 1.

From the anticommutation relations (48) it follows that the trace of each of these matrices vanishes. For example.

$$\alpha_x = -\beta \alpha_x \beta \, \{ : \beta^2 = 1 \Rightarrow \beta^{-1} = \beta \}$$

and by the cyclic property of the trace (Tr AB=Tr BA) we have Tr $\alpha_x = -\text{Tr }\beta\alpha_x\beta = -\text{Tr }\beta^2\alpha_x = -\text{Tr }\alpha_x \Rightarrow \text{Tr. }\alpha_x = 0$.

Since the trace is defined as the sum of all the eigenvalues, the number of positive and negative eigenvalues +1 and -1 must be equal, and the α 's and β must therefore, be even dimensional matrices. The simplest even dimensional matrix may be a 2×2 matrix. Any arbitrary 2×2 matrix can be expressed as a linear combination of the Pauli matrices σ_{α} , σ_{y} , σ_{z} and the 2×2 unit matrix $I_{2\times 2}$ (see problem 19 (d) of chapter-3). Pauli matrices satisfy the equation

$$\sigma_x \sigma_y = -\sigma_y \sigma_x = i\sigma_z, \qquad \dots (54)$$

together with two similar relations obtained by permuting x, y, z, But it is impossible to find a fourth matrix which anticommutes

[†] In his orginal paper, Dirac choose to use the negative sign in the eqn. (51)

with all the σ 's. Thus the two dimensional matrices α 's and β are not possible.

The smallest dimension in which the α 's and β can be realized is four, and that is the case we shall study new. In a particular explicit representation the matrices are:

 $\alpha_{x} = \begin{pmatrix} 0 & \sigma_{x} \\ \sigma_{x} & 0 \end{pmatrix}; \ \alpha_{y} = \begin{pmatrix} 0 & \sigma_{y} \\ \sigma_{y} & 0 \end{pmatrix}; \ \alpha_{z} = \begin{pmatrix} 0 & \sigma_{z} \\ \sigma_{z} & 0 \end{pmatrix} \text{ and } \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$...(55)†

where σ_x , σ_y and σ_z are the Pauli spin matrices and I is the 2×2 unit matrix.

Charge and Current Densities. We have the Dirac equation as:

$$(-i\hbar c\alpha. \nabla + \beta mc^2) \psi = i\hbar \frac{\partial \psi}{\partial t}.$$
 (56)

Taking the Hermitian conjugate of (56), we get

$$i\hbar c \nabla \psi \dagger .\alpha + \psi \dagger \beta mc^2 = -i\hbar \frac{\partial \psi \dagger}{\partial t}$$
 ...(57)

$$\{ : \overrightarrow{\alpha \dagger} = \overrightarrow{\alpha}; \beta \dagger = \beta \text{ and } \nabla \dagger = -\nabla \},$$

Multiplying (56) from left by $\psi \uparrow$ and (57) from right by ψ , we obtain

$$-i\hbar c\psi \dagger \alpha. \nabla \psi + mc^2 \psi \dagger \beta \psi = i\hbar \psi \dagger \frac{\partial \psi}{\partial t}, \qquad ...(58)$$

$$i\hbar c \nabla \psi \dagger .\alpha \psi + mc^2 \psi \dagger \beta \psi = -i\hbar \frac{\partial \psi \dagger}{\partial t} \psi.$$
 ...(59)

Subtracting (58) from (59), we get

$$i\hbar \frac{\partial (\psi \dagger \psi)}{\partial t} + i\hbar c \nabla \cdot (\psi \dagger \alpha \psi) = 0$$

$$\frac{\partial P(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{S}(\mathbf{r}, t) = 0, \qquad \dots (60)$$

or

where we recognize the probability and current densities as

$$P(\mathbf{r}, t) = \psi \dagger \psi \qquad \dots (61)$$

$$S(\mathbf{r}, t) = c \psi \dagger \alpha \psi.$$

Expression for the probability has the familiar form and it is never negative. It can very well be interpreted as the position probability density. The current density expression looks more plausible if we note that $c \propto i$ is the velocity of the particle in the usual sense:

[†]There may be many other choices for the 4×4 matrices, but it is customary to deal with this choice after to Dirac.

if
$$\frac{d\mathbf{r}}{dt} = [\mathbf{r}, H] = [\mathbf{r}, \alpha \cdot \mathbf{p}c + \beta mc^2] = i \hbar c \alpha$$
.

$$\frac{d\mathbf{r}}{dt} = c \alpha.$$

FREE PARTICLE OR PLANE WAVE SOLUTIONS OF 10.5.

Since α and β are represented by 4×4 matrices, the wavefunction ψ itself must be a column vector as:

$$\psi(\mathbf{r}, t) = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \dots (63)$$

Using it in the Dirac equation with the explicit form of the matrices α_x , α_y , α_z and β , we have

 $(c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2) \psi = E\psi,$

$$\begin{cases}
cp_x \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} + cp_y \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix} + cp_z \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + cp_z \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

$$+mc^{2}\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}\begin{bmatrix}\psi_{1}\\ \psi_{2}\\ \psi_{3}\\ \psi_{4}\end{bmatrix} = E\begin{pmatrix}\psi_{1}\\ \psi_{2}\\ \psi_{3}\\ \psi_{4}\end{bmatrix}$$

or
$$\begin{bmatrix} mc^{2} & 0 & cp_{z} & c(p_{x}-ip_{y}) \\ 0 & mc^{2} & c(p_{x}+ip_{y}) & -cp_{z} \\ c(p_{x}+ip_{y}) & -cp_{z} & 0 \\ -cp_{z} & c(p_{x}-ip_{y}) & -mc^{2} \\ 0 & -mc^{2} \end{bmatrix} \begin{pmatrix} \psi_{1} \\ \psi_{2} \\ \psi_{3} \\ \psi_{4} \end{pmatrix}$$

$$=E\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}.$$

This is equivalent to the following four simultaneous partial differential equations of first order which are homogeneous and linear in ψ 's:

$$\begin{array}{ll}
mc^{2} \psi_{1} + cp_{z} \psi_{3} + c \left(p_{x} - ip_{y} \right) \psi_{4} = E\psi_{1} & ...(a) \\
mc^{2} \psi_{2} + c \left(p_{x} + ip_{y} \right) \psi_{3} - cp_{z} \psi_{4} = E\psi_{2} & ...(b) \\
cp_{z} \psi_{1} + c \left(p_{x} - ip_{y} \right) \psi_{2} - mc^{2} \psi_{3} = E\psi_{3} & ...(c) \\
c \left(p_{x} + ip_{y} \right) \psi_{1} - cp_{z} \psi_{2} - mc^{2} \psi_{4} = E\psi_{4} & ...(d)
\end{array} \right\}$$

$$\begin{array}{ll}
...(64)$$

Now the plane wave solutions are of the form

$$\psi_j(\mathbf{r}, t) = u_j \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]; j = 1, 2, 3, 4, ...(65)$$

where u_i 's are numbers. Solutions (65) are the eigenfunctions of the energy operator E and momentum operators p_x , p_y , p_z with eigenvalues $\hbar \omega$ and $\hbar k$, respectively.

Substituting (65) into (64), we get the following set of algebraic equations for u_j 's, where $\hbar \omega = E$ and $\hbar k = p$ are now numbers which are the eigenvalues of the operators E and p:

$$(E - mc^{2}) u_{1} + 0 u_{2} - cp_{z}u_{3} - c (p_{x} - ip_{y}) u_{4} = 0 ...(a)$$

$$0 u_{1} + (E - mc^{2}) u_{2} - c (p_{x} + ip_{y}) u_{3} + cp_{z} u_{4} = 0 ...(b)$$

$$-cp_{z}u_{1} - c (p_{x} - ip_{y}) u_{2} + (E + mc^{2}) u_{3} + 0 u_{4} = 0 i...(c)$$

$$-c (p_{x} + ip_{y}) u_{1} + cp_{z}u_{2} + 0 u_{3} + (E + mc^{2}) u_{4} = 0 ...(d)$$
...(66)

It is a set of four homogeneous equations in u_1 , u_2 , u_3 and u_4 . For a non-trivial solution we should have the determinant of the matrix of coefficients as zero, *i.e.*

$$\begin{vmatrix} (E-mc^{2}) & 0 & -cp_{z} & -c(p_{x}-ip_{y}) \\ 0 & (E-mc^{2}) & -c(p_{x}+ip_{y}) & cp_{z} \\ -cp_{z} & -c(p_{x}-ip_{y}) & (E+mc^{2}) & 0 \\ -c(p_{x}+ip_{y}) & cp_{z} & 0 & (E+mc^{2}) \end{vmatrix} = 0.$$

On evaluating the determinant we get

$$(E^2 - m^2c^4 - c^2p^2)^2 = 0. ...(67)$$

From (67), we get the correct relation between the energy and the momentum. Explicit solutions can be obtained for any momentum p by choosing a sign for energy E. Taking $E=E_+$ $=\sqrt{(c^2p^2+m^2c^4)}$, we find that out of four equations (66) only two are linearly independent*. Thus we can solve these only for two of u_1 , u_2 , u_3 and u_4 in terms of the other two, which may be taken arbitrarily. For convenience, taking $u_1=1$ and $u_2=0$, we find that,

$$u_3 = \frac{cp_z}{E_+ + mc^2}$$
 and $u_4 = \frac{c(p_x + ip_y)}{E_+ + mc^2}$...(68a)

and if we take $u_1=0$ and $u_2=1$, then

and

$$u_3 = \frac{c (p_x - ip_y)}{E_+ + mc^2}$$
 and $u_4 = \frac{-cp_z}{E_+ + mc^2}$(68b)

*To see it, let us consider the special case in which the momentum of the particle is zero, i.e. the particle is at rest. Then $E=E_{+}=mc^{2}$ and hence we have $(E-mc^{2})=0$ and $E+mc^{2}=2mc^{2}$, Then it is seen that in equations (66),

$$(a) = c (p_x - ip_y) \times (c) + cp_z \times (d)$$

$$(b) = -c (p_x + ip_y) \times (d) \rightarrow cp_z \times (c).$$

So we see that (a) and (b) can be expressed in terms of (c) and (d) i.e, only (c) and (d) are linearly independent.

Solutions (68a and b) forms a complete set of solutions for positive energy and any other solution for positive energy can be expressed as linear combination of these solutions.

Similarly, for the negative energy $E=E_-=-\sqrt{(c^2p^2+m^2c^4)}$, we obtain two new solutions, which are conveniently written as:

$$u_1 = \frac{cp_z}{E_- - mc^2}, u_2 = \frac{c(p_x + ip_y)}{E_- - mc^2}, u_3 = 1, u_4 = 0$$
 .. (69a)

and

$$u_1 = \frac{c (p_x - ip_y)}{E_- - mc^2}, u_2 = \frac{-cp_z}{E_- - mc^2}; u_3 = 0, u_4 = 1.$$
 ...(69a)

our linearly independent solution.

The four linearly independent solutions are thus given by.

$$u^{1}(\mathbf{p}) = \begin{bmatrix} 1 \\ 0 \\ \frac{cp_{z}}{E_{+} + mc^{2}} \\ \frac{c(p_{x} + ip_{y})}{E_{+} + mc^{2}} \end{bmatrix}, \quad u^{2}(\mathbf{p}) = \begin{bmatrix} 0 \\ 1 \\ \frac{c(p_{x} - ip_{y})}{E_{+} + mc^{2}} \\ \frac{-cp_{z}}{E_{+} + mc^{2}} \end{bmatrix}$$

$$v^{1}(\mathbf{p}) = \begin{bmatrix} \frac{cp_{z}}{E_{-} - mc^{2}} \\ \frac{c(p_{x} + ip_{y})}{E_{-} - mc^{2}} \\ 1 \\ 0 \end{bmatrix} \text{ and } v^{2}(\mathbf{p}) = \begin{bmatrix} \frac{c(p_{x} - ip_{y})}{E_{-} - mc^{2}} \\ \frac{-cp_{z}}{E_{-} - mc^{2}} \\ 0 \\ 1 \end{bmatrix}$$

$$u^{2}, v^{1}, v^{2} \text{ in the above } v^{2}$$

 u^1 , u^2 , v^1 , v^2 in the above are known as the Dirac Spinors. u^r (p); r=1, 2 are the positive energy spinors which describe respectively the particles with spin up and spin down. $v^r(p)$; r=1, 2are negative energy spinors with spin up and spin down. Solution of the Dirac equation for a free particle is thus given from (65) as the Dirac Spinors multiplied by exp. $\{i (k \circ r - \omega t)\}$.

In the non-relativistic limit, the velocity 'v' of the particle is much smaller than the velocity of light, i.e. $c \mid \mathbf{p} \mid << mc^2$, and $E_{+} = -E_{-} \cong mc^{2}$. For positive energy spinors, u_{3} and u_{4} are of the order of v/c times u_1 or u_2 , i.e., the first two components in u^1 and u² are the large components while the last two components are small components. Opposite is true for the negative energy spinors. In the limiting case of the particle at rest (p=0), the four spinors have the simple form:

Energy
$$E: \frac{+mc^2}{+mc^2} + \frac{+mc^2}{-mc^2} - \frac{-mc^2}{-mc^2}$$

Spinor: $u^1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}; u^2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}; v^1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } v^2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}...(70)$

Spin: \uparrow

Orthonormality and Completeness Relations for Spinors. For a particle confined in a cube of side L and volume V, we can write the plane wave solutions of the Dirac equation as

$$\psi(\mathbf{r}, t) = \frac{1}{\sqrt{(V)}} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} \exp\{i(\mathbf{p} \cdot \mathbf{r} - E_p t)/\hbar\}, \dots (71)$$

where $p=\hbar k$ is the momentum and $E_p=\hbar \omega$ is the energy of the particle.

For the positive energy states, we have

$$\psi(\mathbf{r}, t) = \frac{1}{\sqrt{(V)}} u^r(\mathbf{p}) \exp\{i(\mathbf{p} \cdot \mathbf{r} - E_p t)/\hbar\}.$$
 ...(72a)

and similarly for the negative energy states

$$\psi(\mathbf{r}, t) = \frac{1}{\sqrt{(V)}} v^r(\mathbf{p}) \exp \{i (\mathbf{p} \cdot \mathbf{r} + E_p t)/\hbar\}.$$
 ...(72b)

Substituting (72a and b) into the Dirac equation (53), we get the equations satisfied by the spinors u^r and v^r as

$$(c \stackrel{\rightarrow}{\alpha} \cdot \mathbf{p} + \beta mc^2) u^r (\mathbf{p}) = E_p u^r (\mathbf{p}), \qquad ...(73a)$$

and

$$(c \overset{\frown}{\alpha} \cdot \mathbf{p} + \beta mc^2) v^r (\mathbf{p}) = -E_p v^r (\mathbf{p}). \qquad ...(73b)$$

Taking the Hermitian conjugate of equations (73), we get

$$u^r\dagger$$
 (p) $(c \alpha \cdot \mathbf{p} + \beta mc^2) = E_p u^r\dagger$ (p), ...(74a)

$$v^r \dagger (\mathbf{p}) \stackrel{\rightarrow}{(c \alpha \cdot \mathbf{p} + \beta mc^2)} = -E_p v^r \dagger (\mathbf{p}).$$
 ...(74b)

Multiplying (73a) by $u^r \dagger \beta$ from the left, and (74a) by βu^r from the right, and adding the two we obtain

$$2mc^2u^r \dagger u^r = 2E_p u^r \dagger \beta u^r, \qquad ...(75)$$

because α and β anticommute. Defining the adjoint of u by $\ddot{u}=u^{\dagger}\beta$, we write (75) as

$$u^r \dagger u^r = \frac{E_p}{mc^2} \, \overline{u}^r u^r. \tag{76}$$

It is advantageous to normalize the Dirac spinors per volume mc^2/E_p rather then per unit volume. Because, if we start with a unit volume when the particle is at rest, then it will be reduced by the Lorentz-Fitzgerald contraction to

$$\sqrt{\left(1-\frac{v^2}{c^2}\right)} = \frac{mc^2}{E_p}$$

in the direction of motion, when the particle is moving with a

Hence the probability density per unit volume 'u' †u''
velocity v.

Velocity be invariant. By defining the normalization velocity v.

Velocity v.

By defining the normalization per volume will not be invariant. By defining the normalization per volume will not we see from (76) that the probability density will not be see from (76) that the probability density acquires the mc^2/E_p , we see from (76) that the probability density acquires the factor E_p/mc^2 to compensate for the Lorentz mc^2/E_p , we say acquires the mc^2/E_p , we factor E_p/mc^2 to compensate for the Lorentz contraction. Therefore we take

 $u^r \dagger u^r = \frac{E_p}{mc^2}.$.. (77a)

Using it in (76) we find that

$$\bar{u}^r \ u^r = 1 \qquad \dots (78a)$$

Similarly for the negative energy spinors, we have from equations (73b) and (74b) that

$$v^{r} \dagger v^{r} = \frac{-E_{p}}{mc^{2}} \bar{v}^{r} v^{r}$$
 .. (79)

The normalization demands

$$v^r \dagger v^r = \frac{E_p}{mc^2} \qquad \dots (77b)$$

From which,

$$\overline{v^r} \ v^r = -1 \qquad \qquad \dots \tag{78b}$$

Next we consider the orthogonality relations for the spinors. $u^r(p)$ are two positive energy spinors which are the eigenfunctions of the same Hermitian operator, c α. p+βmc². Hence we can always choose them to be orthogonal to each other and hence the orthonormality condition for them becomes:

$$\bar{u}^r$$
 (p) $u^s(p) = \delta_{rs} (r, s=1, 2)$...(79a)

Similarly, for the negative energy spinors v^r (p) we have:

$$\overline{v}^r$$
 (p) v^s (p)= $-\delta_{rs}$ (r, s=1, 2) ...(79b)

Furthermore, we can easily show that the solutions ur (p) and v^r (p) are orthogonal to each other. For it we have

$$(c \alpha \cdot \mathbf{p} + \beta mc^2) u^r (\mathbf{p}) = E_p u^r (\mathbf{p}),$$

and

$$v^{s\dagger}$$
 (p) $(c \stackrel{\rightarrow}{\alpha} \cdot \mathbf{p} + \beta \ mc^2) = -E_p v^{s\dagger}$ (p)

Multiplying first of these equations by $u^s \dagger \beta$ from the left and the second equation by βu^r from the right and adding, we get:

$$2 mc^2 \overline{v}^s (p) \mu^r (p) = 0 \Rightarrow \overline{v}^s (p) u^r (p) = 0 (r, s = 1, 2).$$
 ...(80)

Similarly it can be shown that:

$$\overline{u}^{s}$$
 (p) v^{r} (p)=0 $(r, s=1, 2)$...(81)

Because of the orthogonality and the normalization relations, the Dirac spinors satisfy the following completeness relation:

$$\sum_{r=1}^{2} \{ u_{\alpha}^{r} (\mathbf{p}) \overline{u}_{\beta}^{r} (\mathbf{p}) - v_{\alpha}^{r} (\mathbf{p}) \overline{v}_{\beta}^{r} (\mathbf{p}) \} = \delta_{\alpha\beta} \qquad \dots (82)$$

The minus sign in the above arises due to normalization (78b) for the negative energy solutions.

Interpretation of Negative Energy Solutions. In Dirac theory, the ground state of an atom is not the lowest state since there exists a continuum of negative energy states from $-mc^2$ to $-\infty$. If an atomic electron with energy greater than $+mc^2$ emits spontaneously a photon of energy greater than $2mc^2$ and falls into a negative energy state, it will keep on lowering its energy by emitting photons since there is no lower bound to the negative energy states. Since the ground state is stable, such catastrophic transitions are not at all physical.

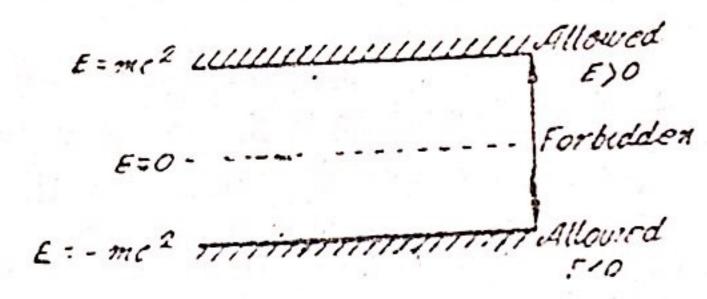


Fig. 1.

In order to remove this difficulty, Dirac proposed that all the negative energy states are completely filled under normal conditions and due to Pauli's exclusion principle transition into these occupied states is prevented. The Dirac sea of completely filled negative energy states is termed as the vacuum. Though the positive energy electrons cannot be transited to the completely filled negative states, there is no restriction for a negative energy electron to absorb a photon of energy greater than $2mc^2$ and become an E>0 state. Consequently, a 'hole' is created in the Dirac sea. The hole is a particle of charge +e and positive energy. Anderson, in 1932, actually discovered such a particle, called the positron.

Let us examine it a little more closely. The absorption of a photon of sufficient energy by a negative energy electron, will escalate it to a positive energy state, i.e.,

$$e^-E<0$$
 +Photon $\rightarrow e^-E>0$

According to hole-theory, this appears as

Photon
$$\to e^-_{E>0} + e^+_{E>0}$$

Although a photon cannot produce an electron positron pair in free space without violating energy and momentum conservation, it can occur in the Coulomb field of a nucleus (pair production). On the other hand, if a positive energy electron fills a hole we have disappearance of the electron and positron as particles with emission of photon of energy $\geq 2mc^2$ (pair annihilation). Both of these processes have been observed experimentally.

10.6. SPIN OF THE ELECTRON:

As we mentioned earlier, the Dirac equation automatically accommodate the spin of the electron. To prove it we write the Hamiltonian for a Dirac particle in the presence of potential V(r) as:

$$H = c \stackrel{\rightarrow}{\alpha} \cdot \mathbf{p} + \beta mc^2 + V(r). \qquad ...(83)$$

Since the potential is assumed to be central, we might expect that the orbital angular momentum $L=r\times p$ is a constant of motion. To investigate this, let us calculate the time rate of change of L in the Heisenberg representation. Considering the x-component of L we have:

$$i\hbar \frac{dL_x}{dt} = [L_x, H] = [(yp_z - zp_y), (c \alpha \cdot \mathbf{p} + \beta mc^2 + V(r)] \quad .. \quad (84)$$

Since x, y, z and p_x , p_y , p_z commute with α and β , and also in polar coordinates, L_x is a function of $\theta \& \phi$ only, while the central potential V(r) does not depend on $\theta \& \varphi$, and hence L_x also commutes with V(r). Thus we have

$$i \ln \frac{dL_x}{dt} = c\{(yp_z - zp_y) (\alpha_x p_x + \alpha_y p_y + \alpha_z p_z)$$

$$-(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z) (yp_z - zp_y)\}$$

$$= c\{\alpha_y p_z (yp_y - p_y y) - \alpha_z p_y (zp_z - p_z z)\}$$

$$= -i \ln c(\alpha_z p_y - \alpha_y p_z) \neq 0.$$
(85)

Hence the orbital angular momentum is not a constant of motion in Dirac theory. However, we expect on physical grounds that it should be possible to define a total angular momentum which is a constant of motion in a central field. This means that we must find another operator such that the commutator of its x-component with H gives the negative of (85). The sum of this operator with L is then a constant of motion and can be inter-

preted as the total angular momentum. It is not difficult to find such an operator:

if
$$\frac{d\sigma_{x'}}{dt} = [\sigma_{x'}, H] = [\sigma_{x'}, c\rho_{1}(\sigma' \cdot \mathbf{p}) + \beta mc^{2} + V(r)],$$

$$\begin{cases} \text{where } \rho_{1} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \text{ with } I \text{ as the } 2 \times 2 \text{ unit matrix,} \\ \text{and } \rho' = \begin{pmatrix} \overrightarrow{\sigma} & 0 \\ 0 & \overrightarrow{\sigma} \end{pmatrix} \text{ so that } \rho_{1} \overrightarrow{\sigma'} = \begin{pmatrix} 0 & \overrightarrow{\sigma} \\ \overrightarrow{\sigma} & 0 \end{pmatrix} = \alpha \end{cases}$$

Of
$$i \uparrow \frac{d\sigma_{x'}}{dt} = c\rho_1 \{\sigma_{x'} (\sigma_{y'} p_y + \sigma_z p_z) - (\sigma_{y'} p_y + \sigma_{z'} p_z) \sigma_{x'}\}$$

$$= c\rho_1 \{(\sigma_{x'} \sigma_{y'} - \sigma_{y'} \sigma_{x'}) p_y + (\sigma_{x'} \sigma_{z'} - \sigma_{z'} \sigma_{x'}) p_z\}$$

$$= c\rho_1 \{2i\sigma_z p_y - 2i\sigma_{y'} p_z\}$$

$$= 2ic \rho_1 (\sigma_{z'} p_y - \sigma_{y'} p_z)$$

$$= 2ic (\alpha_z p_y - \alpha_y p_z)$$

$$= 2ic (\alpha_z p_y - \alpha_y p_z)$$

$$\vdots \quad \alpha = \rho_1 \quad \sigma_1 \quad \sigma_2 \quad \alpha_2 p_z$$

From (85) and (86), we have

$$\left(\frac{dL_x}{dt} + \frac{1}{2} \hbar \frac{d\sigma x'}{dt}\right) = 0 \qquad ...(87)$$

Thus $(L_x + \frac{1}{2} \hbar \sigma_x')$ is a constant of motion and not L_x . We refer $(L+\frac{1}{2}\hbar \sigma')$ as the total angular momentum, which is conserved. It is the sum of orbital angular momentum L and spin angular momentum

$$S = \frac{1}{2} \hbar \sigma' \qquad ...(88)$$

Hence Dirac equation automatically endows the electron with the spin 1, previously ascribed to a hypothetically spinning motion of the electron.

10.7. MAGNETIC MOMENT OF AN ELECTRON:

It is for many applications convenient to express the four component Dirac function in terms of two component functions

$$\psi_{A} = \begin{pmatrix} \psi_{1} \\ \psi_{2} \end{pmatrix} \text{ and } \psi_{B} = \begin{pmatrix} \psi_{8} \\ \psi_{4} \end{pmatrix} \dots (89)$$

$$\sigma_x \sigma_y = -\sigma_y \sigma_x = i\sigma_z$$

as:

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \tag{90}$$

In terms of (90) and the 2×2 Dirac matrices (55), the free particle Dirac equation can be written as:

$$c \begin{pmatrix} 0 & \overrightarrow{\sigma \cdot \mathbf{p}} \\ \rightarrow & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} mc^2 \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \qquad \dots (91)$$

Now we consider the nonrelativistic limit of the Dirac equation for an electron of charge e interacting with an electromagnetic field (A, φ) . The interaction of the electron with the e.m. field is incorporated by the standard prescription:

$$p \rightarrow p - \frac{e}{c}$$
 A and $E \rightarrow E \cdot ep$...(92)

Hence the Dirac equation in the presence of the e.m. field can be written as:

$$c \begin{pmatrix} 0 & \sigma \cdot (\mathbf{p} - e/c \ \mathbf{A}) \\ \rightarrow \sigma \cdot (\mathbf{p} - e/c \ \mathbf{A}) \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} mc^2 \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = (E - e\varphi) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Defining $\pi = (p - e/c A)$, we can write it as

$$\overrightarrow{c} \stackrel{\rightarrow}{\sigma} \stackrel{\frown}{\circ} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + mc^2 \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + e \varphi \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \dots (93)$$

In the nonrelativistic limit, the rest mass energy ' mc^2 ' of the electron is much greater than its kinetic energy and the interaction energy $e\varphi$. Thus we can write

$$\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} \tilde{\psi}_A \\ \tilde{\psi}_B \end{pmatrix} e^{-imc^2t/\hbar}, \qquad \dots (94)$$

where $\tilde{\psi}_A$ and $\tilde{\psi}_B$ are relatively slowly varying functions of time, because their time dependence is given by the kinetic energy of the electron. Substituting (94) into (93), we obtain the nonrelativistic limit of the Dirac eqn. as:

$$c \xrightarrow{\sigma \circ \pi} \begin{pmatrix} \widetilde{\psi}_{B} \\ \widetilde{\psi}_{A} \end{pmatrix} + e \varphi \begin{pmatrix} \widetilde{\psi}_{A} \\ \widetilde{\psi}_{B} \end{pmatrix} - 2mc^{2} \begin{pmatrix} 0 \\ \widetilde{\psi}_{B} \end{pmatrix} = i \hbar \frac{\partial}{\partial t} \left\{ \begin{pmatrix} \widetilde{\psi}_{A} \\ \widetilde{\psi}_{B} \end{pmatrix} \right\} \dots (95)$$

$$\left\{ :: E \to i \hbar \frac{\partial}{\partial t} \right\}$$

It is equivalent to two homogeneous equations:

$$c \stackrel{\rightarrow}{\sigma} \stackrel{\rightarrow}{\psi}_B + e \varphi \stackrel{\sim}{\psi}_A = i \hbar \frac{\partial \tilde{\psi}_A}{\partial I}$$
, and ...(96a)

$$c \stackrel{\rightarrow}{\sigma} \stackrel{\sim}{\pi} \tilde{\psi}_A + e p \tilde{\psi}_B - 2mc^2 \tilde{\psi}_B = i \hbar \frac{\partial \tilde{\psi}_B}{\partial t} \qquad ...(96b)$$

For small kinetic energy and the field interaction energy, we can neglect the terms ih $\frac{\partial \tilde{\psi}_B}{\partial t}$ and $e\varphi \tilde{\psi}_B$ in the comparison with the term $2mc^2 \tilde{\psi}_B$. Thus from (96b), we write

$$c \stackrel{\rightarrow}{\sigma} \stackrel{\rightarrow}{\eta} \tilde{\psi}_{A} - 2mc^{2} \tilde{\psi}_{B} = 0$$

$$\stackrel{\rightarrow}{\tilde{\psi}_{B}} = \frac{\sigma \cdot \pi}{2mc} \tilde{\psi}_{A} \qquad ...(97)$$

or

Inserting (97) into (96a), we obtain a two component spinor equation:

$$i\hbar \frac{\partial \tilde{\psi}_{A}}{\partial t} = \left[\frac{(\vec{\sigma} \cdot \vec{\pi})}{2m} + e\varphi \right] \tilde{\psi}_{A} \qquad ...(98)$$

From the identity, $(\vec{\sigma} \cdot A) (\vec{\sigma} \cdot B) = A \cdot B + i \vec{\sigma} \cdot (A \times B)$ [see problem-9 Chapter-7 we have: ...(99)

$$(\overrightarrow{\sigma} \circ \overrightarrow{\pi}) (\overrightarrow{\sigma} \circ \overrightarrow{\pi}) = \pi^{2} + i \overrightarrow{\sigma} \circ (\overrightarrow{\pi} \times \overrightarrow{\pi})$$

$$\overrightarrow{\pi} \times \overrightarrow{\pi} = \left(\mathbf{p} - \frac{e}{c} \ \mathbf{A} \right) \times \left(\mathbf{p} - \frac{e}{c} \ \mathbf{A} \right) = -\frac{e}{c} (\mathbf{p} \times \mathbf{A} + \mathbf{A} \times \mathbf{p})$$
Now,

$$(\mathbf{p} \times \mathbf{A} + \mathbf{A} \times \mathbf{p})_{x} = p_{y} A_{z} - p_{z} A_{y} + A_{y} p_{z} - A_{z} p_{y}$$

$$= -i \hbar \frac{\partial A_{z}}{\partial y} + i \hbar \frac{\partial A_{y}}{\partial z} = i \hbar (\nabla \times \mathbf{A})_{x} \qquad \dots (100)$$

Since
$$(p_y A_z - A_z p_y) f = -i\hbar \left[\frac{\partial}{\partial y} A_z - A_z \frac{\partial}{\partial y} \right] f$$

$$= -i\hbar \left[A_z \frac{\partial f}{\partial y} + f \frac{\partial A_z}{\partial y} - A_z \frac{\partial f}{\partial y} \right]$$

$$= -i\hbar f \frac{\partial A_z}{\partial y}$$

$$\therefore (p_y A_z - A_z p_y) = -i \hbar \frac{\partial A_z}{\partial y}$$
Similarly,

$$(A_y p_z - p_z A_y) = i\hbar \frac{\partial A_y}{\partial z}$$
, and hence eqn. (100)

Similar relations can be found for the y and the z components of $(p \times A + A \times p)$. Thus

$$(\mathbf{p} \times \mathbf{A} + \mathbf{A} \times \mathbf{p}) = i\hbar \ (\nabla \times \mathbf{A}) = i\hbar \ \mathbf{B} \quad \{ : \mathbf{B} = \text{curl } \mathbf{A} \}$$

$$\therefore \ \pi \times \pi = -\frac{ie\hbar}{c} \ \mathbf{B} \ \text{and} \ (\sigma \cdot \pi) \ (\sigma \cdot \pi) = \left(\stackrel{\rightarrow}{\mathbf{p}} - \frac{e}{c} \mathbf{A} \right)^2 - \frac{e\hbar}{c} \stackrel{\rightarrow}{\sigma} \cdot \mathbf{B}$$

Using it in (98) we obtain

$$i\hbar \frac{\partial \tilde{\psi}_{A}}{\partial t} = \left[\frac{(\mathbf{p} - e/c \, \mathbf{A})^{2}}{2m} - \frac{e\hbar}{2mc} \stackrel{\rightarrow}{\sigma} \cdot \mathbf{B} + e\varphi \right] \tilde{\psi}_{A} \qquad \dots (101)$$

This is known as the Pauli equation. Comparing it with the Schroedinger equation for an electron in the presence of electromagnetic field we see that (101) involves an additional term containing B. The term $\frac{e\hbar}{2mc}$ σ represents the correct magnetic

dipole moment of an electron. The two components of ψ_A suffice to accomodate two spin degrees of freedom of the electron. Thus the correct magnetic moment of the electron corresponding to the gyromagnetic ratio g=2, automatically emerges.

10.8. SPIN ORBIT ENERGY:

Dirac equation in the presence of a central potential V(r) is written as:

$$E\psi = [c \alpha \cdot \mathbf{p} + \beta \ mc^2 + V(r)] \psi \qquad ...(102)$$

From it we have seen that the spin of the electron is automatically incorporated into the theory. We now show that the spinorbit interaction energy is also a consequence of the Dirac equation (102). For it we shall be considering the nonrelativistic limit of the Dirac equation (102). In terms of the two component spinors ψ_A and ψ_B , we can write (102) as:

$$E\begin{pmatrix} \psi_{A} \\ \psi_{B} \end{pmatrix} = c \begin{pmatrix} 0 & \sigma \cdot \mathbf{p} \\ \Rightarrow & 0 \end{pmatrix} \begin{pmatrix} \psi_{A} \\ \psi_{B} \end{pmatrix} + \begin{pmatrix} mc^{2} & 0 \\ 0 & -mc^{2} \end{pmatrix} \begin{pmatrix} \psi_{A} \\ \psi_{B} \end{pmatrix} + V(r) \begin{pmatrix} \psi_{A} \\ \psi_{B} \end{pmatrix}$$

...(103)

In the nonrelativistic limit we write $E=E'+mc^2$, where mc^2 is much greater than the kinetic energy $\frac{p^2}{2m}$ and the potential energy "V(r)". Eqn. (103) can then be written as the two equations:

$$(E'-V) \psi_A - c (\overrightarrow{\sigma}.\mathbf{p}) \psi_B = 0,$$
 ...(104a)

$$(E'+2mc^2-V)\psi_{B}-c(\sigma\cdot\mathbf{p})\psi_{A}=0 \qquad ...(104b)$$

From (104b) we have

$$\psi_B = (E' + 2mc^2 - V)^{-1} c (\sigma.p) \psi_A$$

Substituting it into (104a) we get

$$E' \psi_{A} = \frac{1}{2m} (\overrightarrow{\sigma}. \mathbf{p}) \left(1 + \frac{E' - V}{2mc^{2}} \right)^{-1} (\overrightarrow{\sigma}. \mathbf{p}) \psi_{A} + V \psi_{A} \qquad \dots (105)$$

Since E' and V are much smaller than mc^2 , in the non-relativistic limit, an expansion in powers of $(E'-V)/2mc^2$ upto first order only is a good approximation. Therefore, eqn. (105) reduces to

$$E' \psi_{A} = \frac{1}{2m} \left[\overrightarrow{(\sigma.p)} \overrightarrow{(\sigma.p)} \overrightarrow{(\sigma.p)} \left(1 - \frac{E'}{2mc^{2}} \right) + \frac{1}{2mc^{2}} \overrightarrow{(\sigma.p)} \overrightarrow{V(r)} \overrightarrow{(\sigma.p)} \right] \psi_{A} + V \psi_{A} \qquad ...(106)$$

From (σ, A) $(\sigma, B) = (A \cdot B) + i \sigma$. $(A \times B)$ we have,

$$(\sigma.p)$$
 $(\sigma.p) = (p.p) + i\sigma.(p \times p) = p^2$.

Also,

$$pV = Vp - i\hbar \nabla V \{ :: (pV) f = -i\hbar \nabla (Vf)$$

= $V(-i\hbar \nabla f) + f(-i\hbar \nabla) \}$

$$(\vec{\sigma}.p) \ V(\vec{\sigma}.p) = V(\vec{\sigma}.p)(\vec{\sigma}.p) - i\hbar \ (\vec{\sigma}.\nabla V)(\vec{\sigma}.p)$$

$$= Vp^2 - i\hbar \ (\nabla V).p + \vec{\sigma}.[(\nabla V) \times p]$$

Using these relations, (106) can written as:

$$E' \psi_{A} = \left[\left(1 - \frac{E' - V}{2mc^{2}} \right) \frac{p^{2}}{2m} + V \right] \psi_{A} - \frac{\hbar^{2}}{4m^{2}c^{2}} (\nabla V) \cdot (\nabla \psi_{A}) + \frac{\hbar}{4m^{2}c^{2}} \stackrel{\rightarrow}{\sigma} \cdot [(\nabla V) \times \mathbf{p} \psi_{A}] \quad .. \quad (107)$$

Since V is a spherically symmetric potential, we have

$$\nabla V = \frac{\mathbf{r}}{r} \frac{dV}{dr}$$
 and $(\nabla V) \cdot \nabla = \frac{dV}{dr} \frac{\partial}{\partial r}$

Therefore (107) can be written as:

$$E' \psi_{A} = \left(\frac{p^{2}}{2m} - \frac{p^{4}}{8m^{3}c^{2}} + V - \frac{\hbar^{2}}{4m^{2}c^{2}} \frac{dV}{dr} \frac{\partial}{\partial r} + \frac{1}{2m^{2}c^{2}} \frac{1}{r} \frac{dV}{dr} S.L\right) \psi_{A}$$
...(108)

$$\left\{ : E' = \frac{p^2}{2m} + V \Rightarrow (E' - V) = \frac{p^2}{2m}, S = \frac{1}{2} \hbar \sigma \text{ and } L = r \times p \right\}$$

The first and the third term on the right side of (108) give the nonrelativistic Schroedinger equation. The second term has the nonrelativistic classical relativistic mass correction, which can be the form of the classical relativistic mass correction, which can be the form by expanding the equare root of $E^2 = c^2 p^2 + m^2 c^4$ as:

form ained by expanding the square root of ained by
$$\exp \operatorname{anding} \operatorname{the square} \left(1 + \frac{p^2}{m^2 c^2}\right)^{1/2}$$

$$E = \left(c^2 p^2 + m^2 c^4\right)^{1/2} = mc^2 \left(1 + \frac{p^2}{m^2 c^2}\right)^{1/2}$$

$$\approx mc^2 \left(1 + \frac{p^2}{2m^2 c^2} - \frac{p^4}{8m^3 c^2}\right)$$

$$= mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2}$$

Last term in (108) gives the spin orbit energy, which is seen to appear as an automatic consequence of the Dirac equation. The appear as a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth term is a similar relativistic correction to the potential fourth ter

encies. SEPARATION OF THE EQUATION AND THE 10.9. SEPARATION ATOM PROBLEM:

The Dirac equation for a central field can be separated without any approximation, in the spherical coordinates. To do this we define radial momentum and velocity operators as:

$$p_r = \frac{1}{r} (\mathbf{r} \cdot \mathbf{p} - i\hbar) \text{ and } \alpha_r = \frac{1}{r} (\alpha \cdot \mathbf{r}) \qquad \dots (109)$$

We also define an operator K which is related to the angular momentum \mathbf{L} as:

$$K=\beta (\overrightarrow{\sigma}'.\mathbf{L}+\hbar)$$
 ...(110)

where $\overrightarrow{\sigma}' = \begin{pmatrix} \overrightarrow{\sigma} & 0 \\ 0 & \overrightarrow{\sigma} \end{pmatrix}$ with $\overrightarrow{\sigma}'$ s as the 2×2 Pauli matrices. Let us

now calculate the value

$$\alpha_{r} p_{r} + ir^{-1} \alpha_{r} \beta K = \frac{1}{r} \stackrel{\rightarrow}{(\alpha.r)} \cdot \frac{1}{r} (r \cdot p - i\hbar) + \frac{i}{r^{2}} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\sigma' \cdot L + \hbar)}$$

$$= \frac{1}{r^{2}} \stackrel{\rightarrow}{(\alpha \cdot r)} [(r \cdot p) + i\sigma' \cdot (r \times p)]$$

$$= \frac{1}{r^{2}} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\alpha \cdot p)}$$

$$= \frac{1}{r^{2}} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\alpha \cdot r)} \stackrel{\rightarrow}{(\alpha \cdot p)}$$

of " To " " " Proprie.

$$\begin{cases}
\vdots \quad (\overrightarrow{\alpha} \cdot \mathbf{A}) \quad (\overrightarrow{\alpha} \cdot \mathbf{B}) = \begin{pmatrix} 0 & \overrightarrow{\sigma} \cdot \mathbf{A} \\ \overrightarrow{\sigma} \cdot \mathbf{A} & 0 \end{pmatrix} \begin{pmatrix} 0 & \overrightarrow{\sigma} \cdot \mathbf{B} \\ \overrightarrow{\sigma} \cdot \mathbf{B} & 0 \end{pmatrix} \\
= \begin{pmatrix} \overrightarrow{\sigma} \cdot \mathbf{A}) \quad (\overrightarrow{\sigma} \cdot \mathbf{B}) & 0 \\ 0 \quad (\overrightarrow{\sigma} \cdot \mathbf{A}) \quad (\overrightarrow{\sigma} \cdot \mathbf{B}) \end{pmatrix} \\
\text{Using } (\overrightarrow{\sigma} \cdot \mathbf{A}) \quad (\overrightarrow{\sigma} \cdot \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} + i \quad \overrightarrow{\sigma} \cdot (\mathbf{A} \times \mathbf{B}) \\
\text{into it we get at once,} \\
(\overrightarrow{\alpha} \cdot \mathbf{A}) \quad (\overrightarrow{\alpha} \cdot \mathbf{B}) = (\mathbf{A} \cdot \mathbf{B}) + i \quad \overrightarrow{\sigma}' \cdot (\mathbf{A} \times \mathbf{B}) \end{cases}$$

$$= \frac{1}{r^2} (\alpha_x x + c_y y + \alpha_z z) (\alpha_x x + \alpha_y y + \alpha_z z) (\overrightarrow{\alpha} \cdot \mathbf{p})$$

$$= \frac{1}{r^2} (\alpha_x^2 x^2 + \alpha_x \alpha_y xy + \alpha_x \alpha_z xz + \alpha_y \alpha_x yx + \alpha_y^2 y^2 + \alpha_z \alpha_z yz + \alpha_z \alpha_z xz + \alpha_z \alpha_y zy + \alpha_z^2 z^2) (\overrightarrow{\alpha} \cdot \mathbf{p})$$

$$= \frac{1}{r^2} (x^2 + y^2 + z^2) (\overrightarrow{\alpha} \cdot \mathbf{p}), \text{ because other terms vanish}$$

due to anticommutation relations of a-matrices.

$$\therefore \alpha_r p_r + \frac{i}{r} \alpha_r \beta K = (\alpha \cdot \mathbf{p}) \qquad \dots (111)$$

Using it, the hamiltonian for the Dirac particle in a central field V(r) can be written as:

$$H = c \xrightarrow{\rightarrow} p + \beta mc^2 + V(r) = c \alpha_r p_r + \frac{ic}{r} \alpha_r \beta K + \beta mc^2 + V(r) \qquad ...(112)$$

The eigenvalues of K can be found by squaring equation (110),

$$K^{2} = \beta \stackrel{\rightarrow}{(\sigma' \cdot L + \hbar)} \cdot \beta \stackrel{\rightarrow}{(\sigma' \cdot L + \hbar)} = \stackrel{\rightarrow}{(\sigma' \cdot L + \hbar)^{2}}$$

$$= \stackrel{\rightarrow}{(\sigma' \cdot L)^{2} + 2\hbar} \stackrel{\rightarrow}{(\sigma' \cdot L) + \hbar^{2}}$$

$$= (L + \frac{1}{2}\hbar\sigma')^{2} + \frac{1}{4}\hbar^{2}$$

$$= J^{2} + \frac{1}{4}\hbar^{2}$$

$$\vdots \quad L + \frac{1}{3}\hbar \stackrel{\rightarrow}{\sigma'} \text{ is the total angular momentum } \stackrel{\rightarrow}{J}$$

This means that the eigenvalues of K^2 and J^2 are related to each other by:

 $\hbar^2 k^2 = j (j+1) \hbar^2 + \frac{1}{4} \hbar^2 \Rightarrow k = \pm (j+\frac{1}{2})$

so that k can be ± 1 , ± 2 , ± 3 ,..., and so on.

We now choose a representation in which H and K are diagonal and represented by numbers E and K, respectively. α_r and β can then be represented by Hermitian matrices which satisfy the relations

$$\alpha_r^2 = \beta^2 = 1$$
, $\alpha_r \beta + \beta \alpha_r = 0$.

This can very easily be verified. Such matrices can have two rows and two columns and can be found out to be

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; c_r = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \dots (113)$$

Further, since k is related to the total angular momentum, the angular and spin parts of the wave-functions are fixed by the requirement hat ψ be an eigenfunction of the K operator. Also K commutes with H (see problem 6(c)) and hence the eigenfunction ψ of K is also an eigenfunction of H. For the computation of the energy of the system, only radial part of the wavefunction is needed and the structure of β and α_r in eqn. (113) demands that the radial part has got two components, which we write as

$$\psi_{rad} = \begin{pmatrix} F(r)/r \\ G(r)/r \end{pmatrix} \dots (114)$$

Substituting (114) and (113) into the Dirac equation $H\psi = E\psi$, with the Hamiltonian (112) we get:

$$\begin{cases} -i \ln c \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} + \frac{1}{r} \end{pmatrix} + \frac{ic}{r} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix} \\ + \begin{pmatrix} mc^2 & 0 \\ 0 & -mc^2 \end{pmatrix} + V - E \end{cases} \begin{pmatrix} F(r)/r \\ G(r)/r \end{pmatrix} = 0$$
This is a single factor of the following states as the following states are single factors.

This is equivalent to the following two equations:

$$(E - mc^{2} - V) F(r) + \hbar c \frac{dG(r)}{dr} + \frac{\hbar ck}{r} G(r) = 0, \text{ and}$$

$$(E + mc^{2} - V) G(r) - \hbar c \frac{dF(r)}{dr} + \frac{\hbar ck}{r} F(r) = 0 \qquad ...(115)$$

These equations may be further written as:

$$\left(-\frac{mc^2 - E}{\hbar c} - \frac{V}{\hbar c}\right) F(r) + \frac{dG(r)}{dr} + \frac{k}{r} F(r) = 0 \qquad \dots (116a)$$

and

$$\left(\frac{mc^2 + E}{\hbar c} - \frac{V}{\hbar c}\right) G(r) - \frac{dF(r)}{dr} + \frac{k}{r} F(r) = 0$$
 ...(116b)

Now substituting

$$\frac{mc^2 + E}{\hbar c} = \alpha_1; \frac{mc^2 - E}{\hbar} = \alpha_2; \sqrt{(\alpha_1 \alpha_2)} = \frac{\sqrt{(m^2c^4 - E^2)}}{\hbar c} = \alpha \text{ and } \dot{\rho} = \alpha r$$

Equations (116) read as:

$$\left(\frac{d}{d\rho} + \frac{k}{\rho}\right)G - \left(\frac{\alpha_2}{\alpha} + \frac{V}{\hbar c\alpha}\right)F = 0 \qquad \dots(117a)$$

$$\left(\frac{d}{d\rho} - \frac{k}{\rho}\right)F - \left(\frac{\alpha_1}{\alpha} - \frac{V}{\hbar c\alpha}\right)G = 0 \qquad \dots(117b)$$

Hydrogen atom. We now find energy eigenvalues of equations (117) for the case of a hydrogen atom. The potential for the hy rogen atom is given by

$$V(r) = \frac{-Ze^2}{r} \qquad ...(118)$$

Using (118) into (117) and denoting $Ze^2/\hbar c$ by γ we get the equations to be solved as:

$$\left(\frac{d}{d\rho} + \frac{k}{\rho}\right)G - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho}\right)F = 0 \qquad \dots (119a)$$

$$\left(\frac{d}{d\rho} - \frac{k}{\rho}\right)F\left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho}\right)G = 0$$
 ...(119b)

As in the case of nonrelativistic treatment of hydrogen atom, we seek solutions of the from

$$F = f(P) e^{-P}$$
 and $G = g(P) e^{-P}$...(120)

Substituting these in (119) we obtain:

$$g' - g + \frac{kg}{\rho} - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho}\right) f = 0$$

$$f' - f - \frac{kf}{\rho} - \left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho}\right) g = 0$$
...(121)

To solve these equations for f and g we use the power series method:

$$\begin{cases}
f = \sum_{n} a_{n} \rho^{\varepsilon + n} ; a_{0} \neq 0 \\
g = \sum_{n} b_{n} \rho^{\varepsilon + n} ; b_{0} \neq 0
\end{cases} \qquad \dots (122)$$

where s is so chosen that the solutions F/r and G/r are well behaved at the origin.

Substituting (122) into (121) and equating the coefficients of $\rho^{s+\nu-1}$ to zero, we obtain the following recursion relations:

$$\left\{ (s+\nu+k) \ b_{\nu} - b_{\nu-1} + \gamma a_{\nu} - \frac{\alpha_2}{\alpha} a_{\nu-1} = 0, \\
\text{and} \quad s+\nu-k) \ a_{\nu} - a_{\nu-1} - \gamma b_{\nu} - \frac{\alpha_1}{\alpha} b_{\nu-1} = 0 \right\} \dots (123)$$

when v=0, the equations analogous to (123) are:

and
$$(s+k) b_0 + \gamma a_0 = 0,$$

 $(s-k) a_0 - \gamma b_0 = 0$
...(124)

Equations (124) have the required nonvanishing solution for a_0 and b_0 only if the determinant of their coefficients vanishes:

$$\begin{vmatrix} \gamma \\ s-k \end{vmatrix} = 0 \Rightarrow s = \pm (k^2 - y)^{1/2} \dots (125)$$

From the boundary condition at the origin, the wavefunction must be finite at the origin. For this, s should be positive and music in (125) we take only the positive sing, i.e.,

 $S = (k^2 - \gamma^2)^{1/2}$...(126)

Now to obtain a relation between a_v and b_v we multiply first of equations (123) by α and second by α_2 . Then

$$(s+v+k) \alpha b_v - \alpha b_{v-1} + \alpha \gamma a_v - \alpha_2 a_{v-1} = 0$$

$$(s+v-k) \alpha_2 a_v - \alpha_2 a_{v-1} - \alpha_2 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_2 a_v - \alpha_2 a_{v-1} - \alpha_2 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_3 a_v - \alpha_4 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

$$(s+v-k) \alpha_5 a_v - \alpha_5 a_{v-1} - \alpha_5 \gamma b_v - \alpha b_{v-1} = 0$$

Subtracting one of these equations from the other we get:

$$b_{\nu}[\alpha (s+\nu+k)+\alpha_{2}\gamma]=a_{\nu}[\alpha_{2}(s+\nu-k)-\alpha_{2}\gamma]$$
 ...(127)

The power series solutions at large r is determined by higher power terms, unless both the series terminate. For higher order terms, we can neglect constant factors in comparison to v and write (127) as

$$b_{\nu} \cong \frac{\sigma_2}{\alpha} a_{\nu}$$

Using it in (123), we obtain

$$a_{\nu} \approx \frac{2}{\nu} a_{\nu-1} \text{ and } b_{\nu} \approx \frac{2}{\nu} b_{\nu-1}$$
 ...(128)

Now,
$$e^{2\rho} = \sum_{n=0}^{\infty} \frac{(2\rho)^n}{n!} = \sum_{n=0}^{\infty} C_n \zeta^n \text{ with } C_n = \frac{2^n}{n!} \Rightarrow \frac{C_{\nu}}{C_{\nu-1}} = \frac{2}{\nu}.$$

This means that the series for f and g have the asymptotic from $e^{2\rho}$, and the solution F and G will, therefore, behave like $e^{2\rho} \cdot e^{-\rho} = e^{+\rho}$. Thus the solution blows up at the infinity. In order to get regular solutions, the series must be terminated after a finite number of terms. Suppose that it occurs at v=n', so that $a_{n'+1} = 0$ and $b_{n'+1} = 0$. Then taking v = n'+1, both of eqns. 123 give the relation

$$a_2 a_{n'} = -\alpha b_{n'}$$
; $n' = 0, 1, 2, \dots$...(129)

To obtain the energy levels, we set v=n' in (127) and make use of (129), we get

$$-\frac{\alpha_2}{\alpha} a_{n'} \left[\alpha \left(s+n'+k\right)+\alpha_2\gamma\right] = a_{n'} \left[\alpha_2 \left(s+n'-k\right)-\alpha\gamma\right]$$
or
$$-\frac{\alpha_2^2}{\alpha} \gamma + \alpha\gamma = 2\alpha_2 \left(s+n'\right)$$
or
$$-\frac{\alpha_2^2\gamma + \alpha^2\gamma}{\alpha} = 2\alpha_2 \left(s+n'\right)$$
or
$$2\alpha \left(s+n'\right) = \gamma \left(\alpha_1 - \alpha_2\right)$$

$$\{:: \alpha^2 = \alpha_1\alpha_2\}$$

Using the definition of α_1 and α_2 , we write

$$2 \sqrt{\left(\frac{m^2c^4 - E^2}{\hbar^2c^2}\right)(s+n')} = \gamma \frac{2E}{\hbar c}$$

Squaring both sides,

or

or

or

$$4\frac{m^{2}c^{4} - E^{2}}{\hbar^{2}c^{2}}(s+n')^{2} = 4\frac{\gamma^{2}E^{2}}{\hbar^{2}c^{2}}$$

$$E^{2}\gamma^{2} + E^{2}(s+n')^{2} = m^{2}c^{4}(s+n')^{2}$$

$$E^{2}\left(1 + \frac{\gamma^{2}}{(s+n')^{2}}\right) = m^{2}c^{4}$$

$$E = mc^{2}\left[1 + \frac{\gamma^{2}}{(s+n')^{2}}\right]^{-1/2} \qquad ...(130)$$
Now $(s+n') = n' + (k^{2} - \gamma^{2})^{1/2} = n' + \left[(-j + \frac{1}{2})^{3} - \gamma^{2}\right]^{1/2}$

$$= n' + (-j + \frac{1}{2})\left[1 - \frac{\gamma^{2}}{(-j + \frac{1}{2})^{2}}\right]^{1/2}$$

$$= n' + (-j + \frac{1}{2})\left[1 - \frac{1}{2} - \frac{\gamma^{2}}{(-j + \frac{1}{2})^{2}} - \frac{1}{8} - \frac{\gamma^{4}}{(-j + \frac{1}{2})^{4}}\right]$$

$$= \left[(n' + j + \frac{1}{2}) - \frac{\gamma^{2}}{(-j + \frac{1}{2})} - \frac{1}{8} - \frac{\gamma^{4}}{(-j + \frac{1}{2})^{3}}\right]$$

$$= n - \frac{\gamma^{2}}{(2j + 1)} - \frac{\gamma^{4}}{(2j + 1)^{3}} \qquad ...(131)$$

where $n = n' + j + \frac{1}{2}$ is the total quantum number. Using (131) into (130) we get

$$E \stackrel{\square}{=} mc^{2} \left[1 - \frac{1}{2} \frac{\gamma^{2}}{\left(n - \frac{\gamma^{2}}{2j+1} \right)^{2}} - \frac{3}{8} \frac{\gamma^{4}}{\left(n - \frac{\gamma}{2j+1} \right)^{4}} \right]$$

$$= mc^{2} \left[1 - \frac{\gamma^{2}}{2n^{2}} - \frac{\gamma^{2}}{2n^{2}.n} \cdot \frac{2\gamma^{2}}{(2j+1)} - \frac{3\gamma^{4}}{8n^{4}} \right]$$
or
$$E = mc^{2} \left[1 - \frac{\gamma^{2}}{2n^{2}} - \frac{\gamma^{4}}{2n^{4}} \left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4} \right) \right] ...(132)$$

This formula for the energy levels explains the observed fine structure of the hydrogen spectrum. We see that n=n'+|k| is indeed identical to the familiar principle quantum number in non-relativistic quantum mechanics.

Classification of Energy Levels. We have the relation:

$$n'=n'+j+\frac{1}{2}=n'+|k|$$
 ...(133)

From eigenvalue equation of k we observe that k can be zero, hence for n' > 0, all positive and negative value of k are permissible. However, for n' = 0 a contradiction can arise from the relation

or

$$\frac{b_0}{a_0} = -\frac{\gamma}{s+k}$$
 and $\frac{b_0}{a_0} = -\frac{\alpha_2}{\alpha}$, ...(134)

respectively, since s < |k|. First of these expressions is positive or negative depending on k is negative or positive; whereas, second is always negative. Hence, for n'=0, k can assume only positive integral values.

Uptil now it is observed that j value of a level is equal to $|k| - \frac{1}{2}$. In order to connect l with the level, we must make the non-relativistic approximation that the orbital angular momentum is well defined.

Replacing
$$\beta$$
 by $+1$ and $\overrightarrow{\sigma}$ by $\overrightarrow{\sigma}$ in K , we write

$$hK = h \quad (\overrightarrow{\sigma}. L + h) = 2S \cdot L + h^2 \qquad ...(135)$$
Now
$$J = L + S \Rightarrow 2L \cdot S = J^2 - L^2 - S^2$$

:. $\hbar K = J^2 - L^2 - S^2 + \hbar^2$

From it we have,

$$h \cdot h k = j (j+1) h^2 - l (l+1) h^2 - \frac{1}{2} (\frac{1}{2}+1) h^2 + h^2
k = j (j+1) - l (l+1) + \frac{1}{4}
= \frac{(l+1)}{l-l} \text{ for } j = l + \frac{1}{2}
l - l \text{ for } j = l - \frac{1}{2}$$
...(136)

As an example of energy levels in hydrogen atom, we consider the case n=3. The radial quantum number n' can be 0, 1 or 2 and k can be $\pm (3-n')$ except that k can be only ± 3 , when n'=0. The levels along with their non-relativistic classification are given in the following table:

 n'	k	1	j
0	3	2	5/2 ² D _{5/2}
1	-2	2	3/2 2D _{3/2}
1	2	1	$3/2^{2}P_{3/2}$
2	1	1	$1/2 {}^{2}P_{1/2}$
2	1	0	$1/2 \ ^2S_{1/2}$

According to the expression for energy it is observed that states with same |k| or j have the same energy and energy increases with increasing |k|.

10.10. COVARIANT NOTATION:

Before explaining the meaning of the world "covariant" we first define the Lorentz transformations. If two observers describe the same physical event in two different frames of reference O and O', then the co-ordinates and time used by O will definitely be

different than that of O' to describe the event. The rule which relates the co-ordinates and the time with which observer O describes an event to the co-ordinates and time used by observer O' to describe the same event is known as Lorentz transformations between the two sets of co-ordinates. Introducing the space-time vector x_{μ} with the four components given by $x_1 = x$, $x_2 = y$, $x_3 = z$ and $x_4 = ict$. the most general Lorentz transformation; i.e., omitting space time translations, between the two co-ordinates and time systems may be written as:

$$x'_{\mu} = a_{\mu\nu} x_{\nu},$$
 ...(137)

where the coefficients $a_{\mu\nu}$ depend only upon the relative velocities and spatial orientations of the two reference fromes O and O'. The transformation coefficients satisfy the relations

$$a_{\mu\nu} \ a_{\mu\lambda} = \delta_{\nu\lambda}; \ (a^{-1})_{\mu\nu} = a_{\nu\mu}$$
 ...(138)

$$\therefore x_{\mu} = (a^{-1})_{\mu\nu} x'_{\nu} = a_{\nu\mu} x'_{\nu} \qquad ...(139)$$

Equations (137) to (139) serve as defining relations for both, the proper as well as the improper Lorentz transformations. In the former case the determinant of the transformation matrix satisfy the relation,

$$||a|| = +1$$
 ...(140)

Such transformations can be built up by an infinite succession of infinitesimal transformations. The improper transformations are the discrete transformations of space inversion and time reversal. These cannot be built up from a succession of infinitesimal ones. Their transformation matrix satisfy the relation,

$$||a|| = -1$$
 ...(141)

An equation describing some physical system is called covariant or relativistically invariant if the form of the equation does not change under the Lorentz transformations.

Any quantity transforming in the same way as x_{μ} under Lorentz transformations is known as a four-vector. A four-vector b_{μ} with $\mu=1, 2, 3, 4$ stands for

 $b_u = (b_1, b_2, b_3, b_4) = (b, ib_0)$

where b_1 , b_2 , b_3 are known as the space components and these are real while b_4 known as the time component of b_μ is purely imaginary. In general, the Greek indices μ , ν , λ , etc. run from 1 to 4, whereas the italic indices i, j, k, etc. run from 1 to 3. In the fourvector $x_{\mu} = (x_1, x_2, x_3, x_4) = (\mathbf{r}, ict)$, we shall be using the customary notation x for the position vector r. The scalar product of two four-vectors b_{μ} and c_{μ} is defined by

$$b_{i} c_{i} = b. c = \sum_{i=1}^{3} b_{i} c_{i} + b_{4} c_{4} = b.c - b_{0} c_{0}$$
 ...(143)

It is unchanged under Lorentz transformations, since It is unions, so b', $c'_{\mu} = a_{\mu\nu} b_{\nu} a_{\mu\lambda} c_{\lambda} = \delta_{\nu\lambda} b_{\nu} c_{\lambda} = b_{\nu} c_{\nu} = b \cdot c$ From (139) we have,

$$\frac{\partial}{\partial x'_{\mu}} = \frac{\partial x_{\nu}}{\partial x'_{\mu}} \cdot \frac{\partial}{\partial x_{\nu}} = a_{\mu\nu} \frac{\partial}{\partial x_{\nu}}. \dots (144)$$

Thus the four-gradient $\frac{\partial}{\partial x_{\mu}}$ is a four-vector.

The transformations law for a tensor of rank two under the Lorentz transformations is written as:

 $A'_{\mu\nu} = a_{\mu\lambda} a_{\nu\sigma} A_{\lambda\sigma}$...(145)

Similarly we can write the transformation law for the tensors of higher rank.

A four vector a_{μ} is known as time like if $a^2 = |\mathbf{a}|^2 - a_0^2 < 0$ and it is called space like if $a^2 > 0$. The relativistic energy and relation for a free particle, $E^2 = |\mathbf{p}|^2 c^2 + m^2 c^4$, in terms of the time like energy momentum four-vector, $p_{\mu} = (\mathbf{p}, iE/c)$, now reads:

 $p^2 = \frac{E^2}{c^2} - |\mathbf{p}|^2 = m^2 c^2$

The operator relations $E \rightarrow i\hbar \partial/\partial t$ and $\mathbf{p} = -i\hbar \nabla$ can be written together as:

 $P_{\mu} \rightarrow i \hbar \frac{\partial}{\partial x_{\mu}} \equiv i \hbar \partial_{\mu}$, where $\partial_{\mu} \equiv \frac{\partial}{\partial x_{\mu}}$...(146)

(It should be noted that we donot make any distinction between a covarient and a contravariant vector, nor do we define the metric tensor guy, because these complications are absolutely unnecessary in the special theory of relativity)-

In general, hereafter we shall always use natural units in which action (energy times time) is measured in terms of ħ, and length divided by time is measured in terms of c. Thus, in the natural units, $\hbar = c = 1$. In terms of these units, m_e may not only-mean the electron mass but also any one of the following:

(i) reciprocal length

$$m_{\theta} \left(= \frac{1}{\hbar/m_{\theta} c} \right) = \frac{1}{386 \times 10^{-11}} cm^{-1}.$$

(ii) reciprocal time

$$m_o \left(= \frac{1}{\hbar/m_o c^2} \right) = \frac{1}{1 \cdot 29 \times 10^{-21}} \sec^{-1} \dots (149)$$
(iii) energy

 $m_e (=m_e c^2) = 0.511 \ MeV$

(iv) momentum

$$m_{\theta} (= m_{\theta} c) = 0.511 \ MeV/c$$

In natural units, the fine structure constant is simply given

$$\alpha = \frac{e^2}{4\pi} \cong \frac{1}{137}$$

10 11. COVARIANT FORM OF DIRAC EQUATION:

We have the Dirac equation,

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c \left(\alpha_x \frac{\partial \psi}{\partial x} + \alpha_y \frac{\partial \psi}{\partial y} + \alpha_z \frac{\partial \psi}{\partial z} \right) + \beta mc^2 \psi,$$
or
$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c \left(\partial \psi + \partial \psi + \partial \psi \right)$$

or
$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c \left(\alpha_1 \frac{\partial \psi}{\partial x_1} + \alpha_2 \frac{\partial \psi}{\partial x_2} + \alpha_3 \frac{\partial \psi}{\partial \psi_3} \right) + \beta mc^2 \psi,$$

or
$$i \frac{\partial \psi}{\partial (ict)} = -\left(\alpha_1 \frac{\partial \psi}{\partial x_1} + \alpha_2 \frac{\partial \psi}{\partial x_2} + \alpha_3 \frac{\partial \psi}{\partial x_3}\right) + \frac{\beta mc^2}{i\hbar c} \psi$$

Multiplying it by \beta from left side, we get

$$i\beta \frac{\partial \psi}{\partial x_4} = -\left(\beta \alpha_1 \frac{\partial \psi}{\partial x_1} + \beta \alpha_2 \frac{\partial \psi}{\partial x_2} + \beta \alpha_3 \frac{\partial \psi}{\partial x_3}\right) + \frac{mc}{i\hbar} \psi \qquad \dots (147)$$

Now introducing new matrices y as follows:

$$\gamma_k = -i\beta x_k \ (k=1, 2, 3)$$
 \\ \gamma_4 = \beta \, \tag{148}

we can write the Dirac equation (147) in the form

$$\gamma_{1} \frac{\partial \psi}{\partial x_{1}} + \gamma_{2} \frac{\partial \psi}{\partial x_{2}} + \gamma_{3} \frac{\partial \psi}{\partial x_{3}} + \gamma_{4} \frac{\partial \psi}{\partial x_{4}} + \frac{mc}{\hbar} \psi = 0$$

$$\gamma_{\mu} \frac{\partial \psi}{\partial x_{\mu}} + \frac{mc}{\hbar} \psi = 0$$

or

or in terms of the natural units

$$\gamma_{\mu} \frac{\partial \psi}{\partial x_{\mu}} + m\psi = 0$$

$$(\gamma_{\mu} \partial_{\mu} + m) \psi = 0 \qquad ...(149)$$

or

This is the covariant form of the Dirac equation, and in what follows we shall be using this form. Before actually establishing the covariance of (149) under Lorentz transformation, we study the properties of the matrices γ_{μ} (μ =1, 2, 3, 4) involved in (149).

Using the definition of the α and β matrices, the explicit form of Dirac's γ matrices can be written as

$$\gamma_k = -i\beta\alpha_k = -i\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}$$
; and

 $\gamma_4 = \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$; where σ_k (k=1, 2, 3) are the Pauli spin matrices. There matrices satisfy the following anticommutation rule:

$$\gamma_{\mu}\gamma_{\nu} + \gamma_{\nu}\gamma_{\mu} = 2\delta_{\mu\nu} \qquad ...(150)$$

For instance,

$$\gamma_{1}\gamma_{2}+\gamma_{2}\gamma_{1}=\begin{pmatrix}0&-i\sigma_{1}\\i\sigma_{1}&0\end{pmatrix}\begin{pmatrix}0&-i\sigma_{2}\\i\sigma_{2}&0\end{pmatrix}+\begin{pmatrix}0&-i\sigma_{2}\\i\sigma_{2}&0\end{pmatrix}\begin{pmatrix}0&-i\sigma_{1}\\i\sigma_{1}&0\end{pmatrix}$$
$$\begin{pmatrix}\sigma_{1}\sigma_{2}+\sigma_{2}\sigma_{1}&0\\0&\sigma_{1}\sigma_{2}+\sigma_{2}\sigma_{1}\end{pmatrix}=0$$

and $\gamma_4 \gamma_4 + \gamma_4 \gamma_4 = 2\gamma_4 \gamma_4 = 2\beta^2 = 2$.

From (1:0) we see that

$$\gamma_1^2 = \gamma_2^2 = \gamma_3^2 = \gamma_4^2 = 1$$
 ...(151)

Moreover, from the definition, each of the γ_{μ} 's is seen to be Hermitian and traceless, i.e.,

$$\mu_{\mu}^{\dagger} = \gamma_{\mu} \text{ and } T_{r} \gamma_{\mu} = 0$$
 ...(152)

The product of all the four gamma matrices is often used in the theory and we give it a special symbol

$$\gamma_5 = \gamma_1 \gamma_2 \gamma_3 \gamma_4 \qquad \dots (153)$$

ys is also Hermitian as

 $\gamma_5 \dagger = (\gamma_1 \gamma_2 \gamma_3 \gamma_4) \dagger = \gamma_4 \dagger \gamma_3 \dagger \gamma_2 \dagger \gamma_1 \dagger = \gamma_4 \gamma_3 \gamma_2 \gamma_1 = \gamma_1 \gamma_2 \gamma_3 \gamma_4 = \gamma_5.$

 γ_5 anticommutes with all the γ_{μ} 's, i.e.

$$\gamma_5 \gamma_\mu + \gamma_\mu \gamma_5 = 0 \quad (\mu = 1, 2, 3, 4).$$
 ...(154)

It can at once be seen that $\gamma_5^2=1$. In the particular representation of Dirac matrices, we have

$$\gamma_5 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}. \dots (155)$$

We now define the Adjoin of Dirac equation. For it we take the Hermitian conjugate of (149),

$$\psi\dagger (\gamma_k\partial_k-\gamma_4\partial_4+m)=0 \quad \left\{ \because \quad \partial_4\dagger=\frac{\partial}{\partial x_4*}=\frac{\partial}{-\partial x_4}=-\partial_4 \right\}.$$

Multiplying it by γ_4 from the right side, we get

$$\psi \dagger (\gamma_k \partial_k - \gamma_4 \partial_4 + m) \gamma_4 = 0$$

$$\psi \dagger \gamma_4 (-\gamma_k \partial_k - \gamma_4 \partial_4 + m) = 0 \quad \{ : \quad \gamma_k \gamma_4 = -\gamma_4 \gamma_k \}.$$

Defining the adjoint of ψ by $\psi = \psi \dagger \gamma_4$, we get the adjoint of the Dirac equation (149) as

$$\overline{\psi}(-\gamma_{\mu}\partial_{\mu}+m)=0 \qquad ...(156)$$

where the reverse arrow on ∂_{μ} indicates that it acts on ψ .

Multiplying (149) from the left by ψ and (156) by ψ from the right and then subtracting, we get the equation of continuity,

$$\partial_{\mu} (\psi \partial_{\mu} \psi) = 0$$
 or $\partial_{\mu} j_{\mu} = 0$,

where the four-vector current ju is given by

$$j_{\mu} = \overline{\psi} \, \gamma_{\mu} \psi. \qquad \dots (157)$$

10.12. INVARIANCE OF DIRAC EQUATION UNDER LORENTZ TRANSFORMATION

For the Lorentz invariance of the Dirac equation two conditions must be satisfied. Firstly, there should be an explicit prescription that relates $\psi(x)$ and $\psi'(x')$, where $\psi(x)$ and $\psi'(x')$ are respectively the states of a physical system in two different coordinate frames. Secondly, using the above prescription, we must be able to show that in the Lorentz transformed frame the equation has the same functional relationship as in the original frame, *i.e.*, if under Lorentz transformation, the original state $\psi(x)$ is transformed into $\psi'(x')$ according to the relation:

$$\psi'(x') = S \psi(x),$$
 ...(158)

where S is a 4×4 matrix which depends only on the nature of Lorentz transformation $a_{\mu\nu}$, and it is independent of space-time coordinates, then the Dirac equation (149) should look like.

$$(\gamma_{\mu} \partial_{\mu}' + m) \psi'(x') = 0,$$
 ...(159)

in the transformed frame $\{: m \text{ is an invariant quantity and } \gamma_a\text{'s}$ do not involve space time coordinates}.

We require the transformation between $\psi(x)$ and $\psi'(x')$ to be linear, because the Dirac equation and the Lorentz transformations of the coordinates are both linear. Also, S must have an inverse, so that if in the original frame we know $\psi'(x')$ we may express our original wavefunction $\psi(x)$ in terms of $\psi'(x')$:

$$\psi(x) = S^{-1} \psi'(x'). \qquad ...(160)$$

From $x_{\nu} = a_{\nu\mu} x_{\mu}'$, we have

$$\frac{\partial x_{\nu}}{\partial x_{\mu}'} = a_{\nu\mu} \Rightarrow \partial_{\mu}' = \frac{\partial x_{\nu}}{\partial x_{\mu}'} \cdot \frac{\partial}{\partial x_{\nu}} = a_{\nu\mu} \frac{\partial}{\partial x_{\nu}} = a_{\nu\mu} \partial_{\nu}. \quad ...(161)$$

Using (161) in (159), we can write

$$(\gamma_{\mu} a_{\nu\mu} \partial_{\nu} + m) \psi'(x') = 0$$

$$(\gamma_{\mu} a_{\nu\mu} \partial_{\nu} + m) S\psi(x) = 0.$$

Multiplying it by
$$S^{-1}$$
 from the left hand side we get $S^{-1}(\gamma_{\mu} a_{\nu\mu} \partial_{\nu} + m) S \psi(x) = 0$ $(S^{-1} \gamma_{\mu} S a_{\nu\mu} \partial_{\nu} + m) \psi(x) = 0$

...(162) $a_{\mu\nu}$'s are complex number and therefore commute with S}. Equation (162) should be identical to the original Dirac Equation for the Lorentz invariance. This requires that S should

satisfy the condition

$$S^{-1} \gamma_{\mu} S a_{\nu\mu} = \gamma_{\nu}$$

$$S^{-1} \gamma_{\mu} S = a_{\mu\nu} \gamma_{\nu}$$

$$\dots (163)$$

This is the necessary and sufficient condition for the invariance of the Dirac equation under Lorentz transformations.

Now we find the condition for the invariance of the adjoint of Dirac equation, given by

$$\overline{\psi}(-\partial_{\mu}\gamma_{\mu}+m)=0 \qquad ...(164)$$

From (158),

$$\psi'\dagger (x') = \psi\dagger (x) S \dagger$$

$$\psi'\dagger \gamma_4 = \psi\dagger S \dagger \gamma_4 = \psi\dagger \gamma_4^2 S \dagger \gamma_4 \qquad \{ :: \gamma_4^2 = 1 \}$$

 $\overline{\psi}' = \overline{\psi} \ (\psi_3 \ S \dagger \gamma_3).$ or Similarly from (160), we get

$$\psi = \psi' \gamma_4 (S\dagger)^{-1} \gamma_4.$$
 ...(166)

Using it into equation (164), we obtain

$$\overline{\psi} \gamma_4 (S\dagger)^{-1} \gamma_4 (-\gamma_{\mu} a_{\nu\mu} \partial_{\nu}' + m) = 0 \qquad \{ : \partial_{\mu} = a_{\nu\mu} \partial_{\nu}' \}$$

$$\overline{\psi} \gamma_4 (S\dagger)^{-1} \gamma_4 (-\gamma_{\nu} a_{\mu\nu} \partial_{\mu}' + m) = 0$$

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...(165)

Multiplying it by $\gamma_4S\dagger\gamma_4$ from the right hand side

$$\nabla \gamma_4 (S\dagger)^{-1} \gamma_4 (-\gamma_\nu a_{\mu\nu} \partial'_{\mu} + m) \gamma_4 S\dagger \gamma_4 = 0$$

 $\psi'\left(-\gamma_4\left(S\dagger\right)^{-1}\gamma_4\gamma_{\nu}a_{\mu\nu}\gamma_4S\dagger\gamma_5\partial_{\mu}'+m\right)=0.$ or

For the Lorentz invariance, (167) should be identical to (164) in the primed coordinates, i.e.,

$$\overline{\psi}' [-\gamma, \partial_{\mu}' + m] = 0.$$
 ...(168)

Comparing (167) with (168), the condition for the invariance of the adjoint of Dirac equation is found to be

$$\gamma_{\mu} = \gamma_{4} (S\dagger)^{-1} \gamma_{4} \gamma_{\nu} a_{\mu\nu} \gamma_{4} S\dagger \gamma_{4}$$

$$= \gamma_{4} (S\dagger)^{-1} \gamma_{4} S^{-1} \gamma_{\mu} S \gamma_{4} S\dagger \gamma_{4}$$

$$= \gamma_{4} (S\dagger)^{-1} \gamma_{4} S^{-1} \gamma_{\mu} S \gamma_{4} S\dagger \gamma_{4}$$

$$\{ : S^{-1} \gamma_{\mu} S = a_{\mu\nu} \gamma_{\nu} \}$$

$$= (S \gamma_{4} S\dagger \gamma_{4})^{-1} \gamma_{\mu} (S \gamma_{4} S\dagger \gamma_{4})$$

$$=A^{-1}\gamma_{\mu}A; A=S\gamma_{4}S\dagger\gamma_{4}.$$
 ...(169)

From (169), we see that $A\gamma_{\mu} = \gamma_{\mu} A$; i.e. A commutes with γ_{μ} . Therefore, should be a constant multiple of the unit matrix I 4×4 (See Prob. 12 (vi)). $A = bI = S\gamma_4 S \dagger \gamma_4$

or $S\gamma_4 S\dagger \gamma_4 \gamma_4 = S\gamma_4 S\dagger = b\gamma_4$(170)

Since γ_4 is Hermitian and $(S\gamma_4S\dagger)$ is also Hermitian, it follows from (170) that the constant b must be real.

Noting that $\det(pA) = p^N \det A$, if A is $N \times N$ matrix and p multiplies every element in A, and prescribing a normalization for S such that, $\det S = 1$, we have from (170)

det S. det
$$\gamma_4$$
. det $S\dagger = \det(b\gamma_4) = b^4 \det \gamma_4$
 $\Rightarrow b_4 = 1$ or $b = \pm 1$ 171)

To determine that under what condition b is -1 and when it is -1, we consider

$$S\dagger S = (S\dagger \gamma_2) \ (\gamma_4 S) = b\gamma_4 \ (S^{-1}\gamma_4 S)$$

$$= b\gamma_4 \ (a_{44}\gamma_4 + a_{4k}\gamma_k)$$

$$= b \ (a_{44}I + a_{4k} \ (-i\alpha_k))$$

$$\{ \because \gamma_k = -i\gamma_4 \gamma_k \}.$$

Since $S\dagger S$ is Hermitian and positive definite ($S \neq 0$, det $S \neq 0$), the Tr $S\dagger S > 0$. Because Tr $a_k = 0$, we get

$$Tr S | S = ba_{44} Tr I = 4a_{44} > 0, ...(172)$$

i.e., if $a_{44} \leq -1$, b = -1 and if $a_{44} \geq 1$, b = +1.

Hence from (165), we get

$$\psi'(x') = \overline{\psi}(x) \ 5^{-1} A = \frac{a_{41}}{a_{44}} \overline{\psi}(x) \ S^{-1}.$$
 ...(173)

Form of 'S' for Proper Lorentz Transformations. To find the explicit structure of the S-matrix for proper homogeneous Lorentz transformations we note that a finite transformation of this type can be obtained through repeated applications of infinitesimal transformations. We, therefore, first find the form of S for an infinitesimal proper transformation from the condition (163).

Infinitesimal transformations of the form, $x_{\mu}' = a_{\mu\nu}x_{\nu}$, correspond to matrices:

$$a_{\mu\nu} = \delta_{\mu\nu} + \epsilon_{\mu\nu}, \qquad \dots (174)$$

where $\epsilon_{\mu\nu}$ is an infinitesimal four-tensor of rank two. We express $S(a_{\mu\nu})$ to first order in terms of $\epsilon_{\mu\nu}$ as

$$S(\delta_{\mu\nu} + \epsilon_{\mu\nu}) = I + \epsilon_{\mu\nu} M_{\mu\nu}. \qquad ...(175)$$

Since, under Lorentz transformation, the scalar product is invariant, we must have

$$x_{\mu}'y_{\mu}' = (\delta_{\mu\nu} + \epsilon_{\mu\nu}) (\delta_{\mu\rho} + \epsilon_{\mu\rho}) x_{\nu}y_{\rho} = x_{\mu}y_{\cdot},$$

which, to first order in $\epsilon_{\mu\nu}$, requires $\epsilon_{\mu\nu} = -\epsilon_{\nu\mu}$. Hence $\epsilon_{\mu\nu}$ is antisymmetric. But the product $\epsilon_{\mu\nu}$ $M_{\mu\nu}$ must be symmetric for proper Lorentz transformation and hence $M_{\mu\nu}$ must be antisymmetric (the product of two antisymmetric matrices is symmetric).

As an arbitrary 2×2 matrix can be expressed in terms of σ_x , σ_y , σ_z and I (see prob, 19, chapter 3), similarly an arbitrary 4×4 matrix can be expressed in terms of the sixteen matrices:

$$I_{4\times4}$$
 (one), γ_{μ} (four), γ_{5} (one), $\gamma_{5}\gamma_{\mu}$ (four), and $\sigma_{\mu\nu} = \frac{1}{2i}(\gamma_{\mu}\gamma_{\nu} - \gamma_{\nu}\gamma_{\mu})$

(six). Here, $M_{\mu\nu}$ will be proportional to $\sigma_{\mu\nu}$ only, because it is the sole antisymmetric matrix in the above sixteen matrices. Thus we have $M_{\mu\nu} = \lambda \sigma_{\mu\nu}$, where λ is a constant, and hence

$$S = I + \lambda \epsilon_{\mu\nu} \sigma_{\mu\nu}. \qquad ...(176)$$

Upto first order in $\epsilon_{\mu\nu}$,

$$S^{-1} = I - \lambda \epsilon_{\mu\nu} \sigma_{\mu\nu}. \qquad ...(177)$$

Using (176) and (177) in the condition (163) we write:

$$(I - \lambda \epsilon_{\lambda s} \sigma_{\lambda s}) \gamma_{\mu} (I + \lambda \epsilon_{\lambda s} \sigma_{\lambda s}) = (\delta_{\mu \nu} + \epsilon_{\mu \nu}) \gamma_{\nu}$$

or $\gamma_{\mu} + \lambda \gamma_{\mu} \epsilon_{\lambda s} \sigma_{\lambda s} - \lambda \epsilon_{\lambda s} \sigma_{\lambda s} \gamma_{\mu} = \gamma_{\mu} + \epsilon_{\mu \nu} \gamma_{\nu}$ {neglecting second order terms in $\epsilon_{\mu \nu}$ }

Of
$$\lambda \epsilon_{\lambda s} (\gamma_{\mu} \sigma_{\lambda s} - \sigma_{\lambda s} \gamma_{\mu}) = \epsilon_{\mu s} \gamma_{s} = \epsilon_{\lambda s} \gamma_{\mu \lambda} \gamma_{s} = \frac{1}{2} \epsilon_{\lambda s} (\delta_{\mu \lambda} \gamma_{s} - \delta_{\mu s} \gamma_{\lambda})$$

{: $\delta_{\mu\lambda}\gamma_s = \frac{1}{2}$ ($\delta_{\mu\lambda}\gamma_s - \delta_{\mu,\gamma}\gamma_\lambda$) + $\frac{1}{2}$ ($\delta_{\mu\lambda}\gamma_s + \delta_{\mu s}\gamma_\lambda$), and the product of the second term on the right, which is symmetric, with antisymmetric $\epsilon_{\lambda s}$ vanishes; because the product of a symmetric and an antisymmetric tensor-vanishes.}

or
$$\lambda \left[\gamma_{\mu}, \sigma_{\lambda s} \right] = \frac{1}{2} \left[\delta_{\mu \lambda} \gamma_{s} - \delta_{\mu s} \gamma_{\lambda} \right] \qquad ...(178)$$

Now the L.H.S. of (178) can be simplified further as:

L.H.S. =
$$\lambda \left[\gamma_{\mu}, \frac{1}{2i} \left(\gamma_{\lambda} \gamma_{s} - \gamma_{s} \gamma_{\lambda} \right) \right]$$

= $\frac{\lambda}{2i} \left\{ \gamma_{\mu} \left(\gamma_{\lambda} \gamma_{s} - \gamma_{s} \gamma_{\lambda} \right) - \left(\gamma_{\lambda} \gamma_{s} - \gamma_{s} \gamma_{\lambda} \right) \gamma_{\mu} \right\}$
= $\frac{\lambda}{2i} \left\{ \gamma_{\mu} \gamma_{\lambda} \gamma_{s} - \gamma_{\mu} \gamma_{s} \gamma_{\mu} - \gamma_{\lambda} \gamma_{s} \gamma_{\mu} + \gamma_{s} \gamma_{\lambda} \gamma_{\mu} \right\}$
= $\frac{\lambda}{2i} \left\{ (2\delta_{\mu} \lambda - \gamma_{\lambda} \gamma_{\mu}) \gamma_{s} - (2\delta_{\mu s} - \gamma_{s} \gamma_{\mu}) \gamma_{\lambda} - \gamma_{\lambda} (2\delta_{s\mu} - \gamma_{\mu} \gamma_{s}) + \gamma_{s} (2\delta_{\lambda\mu} - \gamma_{\mu} \gamma_{\lambda}) \right\}$
= $\frac{\lambda}{2i} \left\{ 2\delta_{\mu} \lambda \gamma_{s} - 2\delta_{\mu s} \gamma_{\lambda} - \gamma_{\lambda} (2\delta_{s\mu} + \gamma_{s} (2\delta_{\lambda\mu}) \right\}$
= $\frac{4\lambda}{2i} \left\{ \delta_{\mu} \lambda \gamma_{s} - \delta_{\mu s} \gamma_{\lambda} \right\}$

Comparing it with the right hand side we get:

$$\lambda = \frac{i}{4} \qquad \dots (179)$$

$$: S = I + \frac{i}{4} \epsilon_{\mu\nu} \sigma_{\mu\nu} \qquad \dots (180)$$

Now, as a finite transformation is built up of a number of infinitesimal transformations, the S-matrix for a finite transformation $a_{\mu\nu}$ can be written as:

$$S = \lim_{n \to \infty} \left(I + \frac{i}{4} \frac{a_{\mu\nu}}{n} \sigma_{\mu\nu} \right)^{n}, \text{ where } \epsilon_{\mu\nu} = \lim_{n \to \infty} \frac{a_{\mu\nu}}{n}.$$

$$= \exp. \left\{ i a_{\mu\nu} \sigma_{\mu\nu} / 4 \right\}$$

$$\left\{ \therefore \lim_{n \to \infty} \left(1 + \frac{x}{n} \right)^{n} = e^{x} \right\}$$

$$\vdots \quad \psi'(x') = e^{i a_{\mu\nu} \sigma_{\mu\nu} / 4} \psi(x). \qquad \dots (181)$$

Transformation Matrices for Improper Transformation. The improper transformations are the discrete transformations and there are no infinitesimal transformations which can generate such transformations. Two important types of discrete transformations are the *P*-(space reflection), and the *T*-(time reversal) transformations. Now we find out the explicit form of the transformation matrices for these transformations. We start with the *P*-transformation.

(I) P-transformation. This transformation changes x_1, x_2, x_3 into $-x_1, -x_2, -x_3$; while x_4 remains unchanged, i.e.,

$$x_1 \to x_1' = -x_1$$

and $x_4 \to x_4' = x_4$...(182)

Denoting the transformation matrix for this transformation by P, we write

$$\psi'(x') = P \psi(x); \psi(x) = P^{-1} \psi'(x')$$
 ...(183)

Now we find the actual form of P from the requirement of the invariance of Dirac equation under this transformation.

We write the Dirac equation as:

$$(\gamma_{\mu}\partial_{\mu}+m) \psi(x)=0$$

$$(\gamma_{i}\partial_{i}+\gamma_{4}\partial_{4}+m) \psi(x)=0$$
 ...(184)

01

Using (182) and (183) into it, we get the Dirac eqn. in the primed co-ordinates as:

$$(-\gamma_1 \partial_1' + \gamma_4 \partial_4' + m) P^{-1} \psi'(x') = 0$$

Multiplying it by P from the left side,

490

$$(-P\gamma_i P^{-1} \partial_i' + P\gamma_i P^{-1} \partial_i' + m) \psi'(x') = 0 \qquad \dots (185)$$

For invariance, it should be identical to the equation: $(\gamma_i \partial_i' + \gamma_4 \partial_4' + m) \psi'(x') = 0$

Comparing (185) with (186) we get the conditions to be obe-

yed by Pas:

$$\begin{array}{ccc}
P\gamma_{i} & P^{-1} = -\gamma_{i} \\
P\gamma_{4} & P^{-1} = \gamma_{4}
\end{array}$$
...(187)

From the relations (187) we see that P anticommutes with From From with γ_4 . Clearly, γ_1 satisfies both of these γ_i 's while it commutes with γ_4 . conditions and hence $P = e^{i\xi} \gamma_{A}$

where ets is an arbitrary constant phase factor. Since the phase ...(183)factor is of no physical interest we can take

...(189)

The P is evidently unitary, $P^{-1} = P^{\dagger}$...(190)

We have

$$P \psi(x) = \psi'(x') = \psi'(-x, t) = e^{i\xi} \gamma_i \psi(x, t)$$
 ...(191)

To find the transformation law for ψ (x), we have $\bar{\psi}'(x') = \psi'(x')\dagger \gamma_4 = (\psi\dagger\gamma_4\dagger e^{-i\xi}) \gamma_4$ $=e^{-i\xi}\psi_1(x)\gamma_4\gamma_4$

$$\bar{\psi}'(x') = e^{-i\xi} \bar{\psi}(x) \gamma_4 \qquad ...(192)$$

or

(II) T-transformation. Under this transformation t changes Therefore, we can characterize it by: into-t.

$$\begin{cases} x_i \to x_i' = x_i \\ x_4 \to x_4' = x_4 \end{cases} \dots (193)$$

Denoting the transformation matrix by I for this transformation we have,

$$\psi'(x') = T \psi(x); \psi(x) = T^{-1} \psi'(x') \qquad ...(194)$$

Let us now find the explicit form of T from the requirement of invariance of the Dirac equation (184). Using (193) and (194), we can write the Dirac equation in the primed co-ordinates as:

 $(\gamma_i \partial_i' - \gamma_1 \partial_4' + m) T^{-1} \psi'(x') = 0$ $T \left(\gamma_i \partial_i' - \gamma_4 \partial_4' + m \right) T^{-1} \psi' \left(x' \right) = 0$ 10 ...(195) OL $(T \gamma_i T^{-1} \partial_i' - T \gamma_1 T^{-1} \partial_i' + m) \psi'(x') = 0$

For invariance, it should be identical to (186) and bence we get the conditions for invariance by comparing these eqns. as:

$$T \gamma_{i} T^{-1} = \gamma_{i}$$

$$T \gamma_{4} T^{-1} = -\gamma_{4}$$
...(196)

Clearly, the conditions (196) are satisfied if T is proportional to γ4γ5,

and
$$T \gamma_i T^{-1} = \gamma_4 \gamma_5 \gamma_i \gamma_5 \gamma_4 = -\gamma_4 \gamma_5^2 \gamma_i \gamma_4$$

$$= -\gamma_4 \gamma_i \gamma_4 = +\gamma_4^2 \gamma_i = \gamma_i$$

$$T \gamma_4 T^{-1} = \gamma_4 \gamma_5 \gamma_4 \gamma_5 \gamma_4 = -\gamma_4 \gamma_5^2 \gamma_4^{\gamma_4}$$

$$= -\gamma_4 \gamma_4 \gamma_4 = -\gamma_4.$$

T-TRANSFORMATION FOR THE DIRAC EQUTION IN THE PRESENCE OF E.M. FIELD:

We have defined the energy momentum-four vector $p_{\mu} \equiv (\mathbf{p}, iE)$. Also, defining the four vector $A_{\mu} = (A, i\varphi)$ for the electromegnetic field, we see that the interaction of the electron with the field may be introduced by the transformation:

$$p_{\mu} \rightarrow \{(\mathbf{p} - e\mathbf{A}), i(E - \epsilon \varphi)\} = p_{\mu} - eA_{\mu},$$

or by replacing ∂_{μ} by $(\partial_{\mu} - ie A_{\mu})$, because $p_{\mu} = -i\partial_{\mu}$. Thus the Dirac equation in the presence of the electromagnetic field A_{μ} can be written as:

$$[\gamma_{\mu} (\partial_{\mu} - ieA_{\mu}) + m] \psi = 0$$
or
$$[\gamma_{i} (\partial_{i} - ieA_{i}) + \gamma_{4} (\partial_{4} - ieA_{4}) + m] \psi = 0$$
there

When we apply the T-transformation to this equation, there arises a problem that the transformation remains no longer linear. To see it, under T-transformation we have

$$\begin{array}{ccc}
\partial_i \to \hat{c}_i' = \partial_i; \, \partial_4 \to \hat{c}_4' = -\hat{c}_4 \\
A_i \to A_i' = -A_i; \, A_4 \to A_4' = A_4
\end{array} \right\}, \qquad \dots (198)$$

since A_i is generated by currents which reverse sign when the sense of time is reversed.

Using (198), the equation (197) in the transformed frame can be written as:

Comparing (199) with (197) we find that the Dirac equation in the presence of e.m. field is not invariant under time reversal transformation. This is because we are sticking to the linear transformations only. If we go to nonlinear transformation, the invariance can be achieved. To show it we write (193) as:

$$x_{\mu} \to x_{\mu}' = x_{\mu}^{*}$$
 ...(200)

From it we get:

$$\partial_{\mu} \rightarrow \partial_{\mu}' = \partial_{\mu}^{*}$$
 ...(201)

Now taking the complex conjugate of (197) and using (201) wa can write,

$$[\gamma_{\mu}^{*} (\partial_{\mu}' + ie A_{\mu}^{*}) + m] \psi^{*} (x) = 0$$

$$[\gamma_{\mu}^{*} (\partial_{\mu}' - ie A_{\mu}') + m] \psi^{*} (x) = 0 \qquad ...(202)$$

$$\{ :: A_{\mu} \to A_{\mu}' = -A_{\mu}^{*} \}$$

Defining the transformation matrix B as:

$$\psi'(x') = B \psi^*(x),$$
 ...(203)

we can write (202) as:

$$[\gamma_{\mu}^{*}(\partial_{\mu}'-ie\ A_{\mu}')+m]\ B^{-1}\psi'(x')=0$$

Multiplying it from left by B,

$$[B\gamma_{\mu} * B^{-1} (\partial_{\mu}' - ie A_{\mu}') + m] \psi' (x') = 0 \qquad ...(204)$$

For covariance it should be identical to,

$$[\gamma_{\mu} (\partial_{\mu}' - ie A_{\mu}') + m] \psi'(x') = 0,$$

and hence we should have

$$B \gamma_{\mu} * B^{-1} = \gamma_{\mu}$$
 ...(205)

Eqn. (205) is satisfied by taking B proportional to $\gamma_4\gamma_5\gamma_2$ To obtain the transformation rule for $\bar{\psi}(x)$, we have:

$$\overline{\psi}'(x') = \psi'\dagger(x') \gamma_4 = (B\psi^*)\dagger \gamma_4
= (\psi\dagger)^* B\dagger \gamma_4
= (\overline{\psi} \gamma_4)^* B\dagger \gamma_4
= \overline{\psi}^* \gamma_4^* B\dagger \gamma_4
= \overline{\psi}^* B^{-1} \qquad ...(206)$$

{: $B \sim \gamma_4 \gamma_5 \gamma_2$ is unitary and $\gamma_4 * B\dagger = \gamma_4 B\dagger = B\dagger \gamma_4$ }.

10.13. CHARGE CONJUGATION:

The charge conjugation is a symmetry transformation unlike the P-and T-transformations which are related to Lorentz transformations.

Dirac's theory of electron predicts the existence of its antiparticle "positron". In fact, there corresponds an antiparticle to each particle; because the experience shows that the Nature is rather symmetric w.r.t. the transformation,

$$e \rightarrow -e$$
 ...(207)

We now try to cast the Dirac theory into a form which makes this symmetry between the electron and the positron self-evident, i.e., we want that it should be able to form directly the wave-, function of a positron from that of the missing negative energy electron to which it corresponds.

We first investigate that whether the theory based on the Dirac equation with the sign of eA_{μ} reversed is equivalent to the one based on the original Dirac eqn. The original Dirac equation for an electron in the presence of an e.m. field is given by eqn. (197) as:

$$[\gamma_{\mu} (\partial_{\mu} - ieA_{\mu}) + m] \psi (x) = 0 \qquad ...(208)$$

If we denote the wavefunction of the positron by ψ^c , called the charge conjugate wavefunction, then we want to see that whether there is a prescription which relates ψ^c to ψ so that ψ^c obeys the charge-conjugate Dirac equation

$$[\gamma_{\mu} (\partial_{\mu} + ieA_{\mu}) + m] \psi^{c} = 0 \qquad ...(209)$$

Taking the conjugate of equation (208) we get:

$$\bar{\psi}(x)\left[\gamma_{\mu}\left(-\overleftarrow{\partial}_{\mu}-ieA_{\mu}\right)+m\right]=0$$

Taking its transpose, we obtain

$$\left[\tilde{\gamma}_{\mu}\left(-\partial_{\mu}-ieA_{\mu}\right)+m\right]\tilde{\psi}\left(x\right)=0 \qquad ...(210)$$

If we can find a nonsingular matrix C such that

$$C \tilde{\gamma}_{\mu} C^{-1} = -\gamma_{\mu},$$
 ...(211)

we can write (210) as:

$$C\left[\tilde{\gamma}_{\mu}\left(-\partial_{\mu}-ieA_{\mu}\right)+m\right]C^{-1}C\tilde{\psi}(x)=0$$

or
$$[-\gamma_{\mu}(-\partial_{\mu}-ieA_{\mu})+m]C\tilde{\psi}(x)=0$$

or
$$\left[\gamma_{\mu}\left(\partial_{\mu}+ie\ A_{\mu}\right)+m\right]C\widetilde{\psi}\left(x\right)=0 \qquad ...(212)$$

Comparing it with (209) we find that by defining,

$$\psi^{o} = C \widetilde{\psi}(x), \qquad ... (213)$$

equation (209) is as good as the original Dirac equation (208).

From (211), C must commute with γ_1 and γ_3 and anticommute with γ_2 and γ_4 {: $\gamma_2 = \gamma_2$, $\gamma_4 = \gamma_4$ and $\gamma_1 = -\gamma_1$, $\gamma_3 = -\gamma_3$ }. Thus a suitable choice may be

$$C = \gamma_4 \gamma_2 \qquad \dots (214)$$

Now we consider the transformation of \(\psi^c\). For it we consider

$$\psi^c = C \tilde{\psi}$$

$$\Rightarrow \bar{\psi}^{c} = \tilde{\psi} \tilde{\gamma}_{4} C^{-1} \gamma_{4} = -\tilde{\psi} C^{-1} \gamma_{4} \gamma_{4} = -\tilde{\psi} C^{-1} \qquad ...(215)$$

In order to see the significance of the invariance of Dirac equation w.r.t. charge conjugation, let us consider the effect of this transformation on the charge current density $j_{\mu} = ie \Psi \gamma_{\mu} \Psi$ we have

19-1

$$j_{\mu}^{c} = ie \, \overline{\psi}^{c} \, \gamma_{\mu} \, \psi^{c} = -ie \, \overline{\psi} \, C^{-1} \, \gamma_{1} \, C \overline{\psi}$$

$$= ie \, \overline{\psi} \, \overline{\gamma}_{\mu} \, \overline{\psi} = ie \, (\overline{\psi} \gamma_{\mu} \psi) \neq -j_{\mu},$$

$$= ie \, \overline{\psi} \, \overline{\gamma}_{\mu} \, \overline{\psi} = ie \, (\overline{\psi} \gamma_{\mu} \psi) \neq -j_{\mu},$$
Since the total

contrary to our expectation. Since the total field charge changes contrary to C-transformation, j_{μ} should also change size contrary to C-transformation, j_{μ} should also change sign. The sign under sign the definition of j_{μ} . We cannot have sign under sign the definition of j_{μ} . We cannot have a consistent sign unless we regard ψ and $\bar{\psi}$ as non-commutation of j_{μ} . difficulty incommuting operadifficulty incommuting operadifficulty incommuting operapicture for j_{μ} unless we regard ψ and $\bar{\psi}$ as non-commuting operapicture for j_{μ} the Direction of the picture picture 101 July as non-commuting opera-tors. (It will be clear when we shall quantize the Dirac field in tors. Because, ...(216)

chapter-13). Because,

with $(\gamma_{\mu})_{\alpha\beta}$ antisymmetric, we must antisymmetrize $\bar{\psi}_{\alpha}$ ψ_{β} , i.e., $\bar{\psi}_{\alpha}$ $\psi_{\beta} = \frac{1}{2} (\bar{\psi}_{\alpha} \psi_{\beta} - \psi_{\beta})$

$$\frac{ie}{2} \left[\overline{\psi}_{\alpha} \ \psi_{\beta} = \frac{i}{2} \left[\overline{\psi}_{\alpha} \ (\gamma_{\mu})_{\alpha\beta} \psi_{\beta} - \psi_{\beta} \ (\gamma_{\mu})_{\alpha\beta} \psi_{\alpha} \right] \\
\vdots \qquad \frac{ie}{2} \left[\overline{\psi}_{\alpha} \ (\gamma_{\mu})_{\alpha\beta} \psi_{\beta} - \overline{\psi}_{\beta} \ (\gamma_{\mu})_{\alpha\beta} \psi_{\alpha} \right] \\
= \frac{ie}{2} \left[(\overline{\psi} \ \gamma_{\mu} \ \psi) - (\overline{\psi} \ \gamma_{\mu} \ \psi) \right]$$

Hence we have,

$$j_{\mu}^{c} = \frac{ie}{2} \left[(\overline{\psi}^{c} \gamma_{\mu} \psi^{c}) - (\overline{\psi}^{c} \gamma_{\mu} \psi^{c}) \right]$$

$$= \frac{ie}{2} \left[(\overline{\psi} \gamma_{\mu} \psi) - (\overline{\psi} \gamma_{\mu} \psi) \right] = -j_{\mu},$$

$$= \frac{ie}{2} \left[(\overline{\psi} \gamma_{\mu} \psi) - (\overline{\psi} \gamma_{\mu} \psi) \right] = -j_{\mu},$$
We also find

in accordance with our expectation. We also find that the current j_{+} is a combination of two similar terms. One represents the "particle" and the other represents the corresponding "antiparticle". Charge conjugation replaces particle by antiparticle and vice-versa. Thus the symmetric role of -e and +e is very

10.14. PROJECTION OPERATORS FOR ENERGY AND

The positive and negative energy spinors obey the equations:

and

Using the natural units and the energy momentum four

vector $p_{\mu} = (\mathbf{p}, iE_{p})$, we can write these as:

vector
$$p_{\mu} = (\mathbf{p}, iE_{p})$$
, we can write these divided vector $p_{\mu} = (\mathbf{p}, iE_{p})$, we can write these divided $(i \gamma_{\mu} p_{\mu} + ni) u^{r} (\mathbf{p}) = 0$ and $(i \gamma_{\mu} p_{\mu} + m) v^{r} (\mathbf{p}) = 0$ $\{ : \alpha_{k} = i\beta\gamma_{k} \text{ and } \gamma_{4} = \beta \}$

From eqns. (218) we heve:

$$(m-i\gamma_{\mu}p_{\mu}) u (\mathbf{p}) = \{2m-(m+i\gamma_{\mu}p_{\mu})\} u (\mathbf{p})$$

= $2m u (\mathbf{p})$

or

$$\frac{m - i \gamma_{\mu} p_{\mu}}{2m} u(\mathbf{p}) = u(\mathbf{p}) \qquad ...(219a)$$

And similarly,

$$\frac{m - i \gamma_{\mu} p_{\mu}}{2m} v(\mathbf{p}) = 0 \qquad ...(219b)$$

Thus the operator $\frac{m-i\,\gamma_{\nu}p_{\mu}}{2m}$, when operates on the positive energy spinor gives an eigenvalue +1 while it gives zero when operates on the negative energy spinor. It is called the *projection* operator for positive energy spinor and we denote it by $\Lambda^{(+)}(p)$,

$$\Lambda^{(+)}(p) = \frac{m - i\gamma_{\perp} p_{\perp}}{2m} ...(220a)$$

Similarly, it can be seen that the operator $\frac{m+i\gamma_{\mu}p_{\mu}}{2m}$, when

operates on the negative energy spinor gives an eigenvalue +1, while it gives zero when operates on positive energy spinor. This is the negative energy projection operator and we denote it by $\Lambda^{(-)}(p)$,

$$\Lambda^{(-)}(p) = \frac{m + i \gamma_{\mu} p_{\mu}}{2m} \dots (220b)$$

It can very easily be verified that

ly be verified that ...(221)
$$\Lambda^{(+)}(p) + \Lambda^{(-)}(p) = 1$$

and

$$\{\Lambda^{(\pm)}(p)\}^n = \Lambda^{(\pm)}(p)$$
 ...(222)

{ It can proved by induction. For example, when n=2,

$$\{\Lambda^{(+)}\}^2 = \frac{m^2 - p^2 - 2im\gamma_{\mu}p_{\mu}}{4m^2} = \frac{m - i\gamma_{\mu}p_{\mu}}{2m} = \Lambda^{(+)} p, \text{ because}$$

for a free particle, $p^2 = -m^2$.

Also that,

$$\Lambda^{(+)}(p) \Lambda^{(-)}(p) = \Lambda^{(-)}(p) \Lambda^{(+)}(p) = 0$$
 ...(223)
 $\Lambda^{(+)}(p) \Lambda^{(-)}(p) = \Lambda^{(-)}(p) \Lambda^{(+)}(p) = 0$...eannleteness rela-

We can also define $\Lambda^{(\pm)}(p)$ by using the completeness relation for the spinors:

$$\sum_{r=1}^{2} [u^{r}(\mathbf{p}) \overline{u^{r}}(\mathbf{p}) v^{r}(\mathbf{p}) \cdot \overline{v^{r}}(\mathbf{p})] = I$$

Operating both sides of it by $\Lambda^{(+)}(p)$, we find that

$$\sum_{r=1}^{2} u^{r} (p) \overline{u^{r}} (p) = \Lambda^{(+)} (p) \qquad ...(224a)$$

Similary,

$$-\sum_{r=1}^{2} v^{r} (p) \overline{v}^{r} (p) = \Lambda^{(-)} (p) \qquad ...(224b)$$

In order to see the use and significance of the energy operators, we calculate the transition probability from and initial electron state $u_i^r(\mathbf{p})$ to the final state $u_f^{r'}(\mathbf{p})$. If H' is the perturbation part of the Hamiltonian which causes the above transition, than the probability 'm' will be proportional to the square of the

absolute value of matrix the element $(\bar{u}_f^{r'} H' u_i^r)$; i e., $\left| (\bar{u}_f^{r'} H' u_i^r) \right|^2 \dots (225)$

In many problems we are not interested in spin of the final state We can therefore sum over the spin of two final states

If the initial state is likewise unpolarized, we then average over the initial spin states also. Thus,

From the definition (224a) we can write

$$\sum_{i'=1,2} (u_f^{i'})_{\beta} (\overline{u}_f^{i'})_{\alpha} = (\Lambda_f^{(+)})_{\beta\alpha}$$

$$\therefore w - \frac{1}{2} \left[H' \Lambda_i^{(+)} \gamma_4 H'^{\dagger} \gamma_4 \right]_{\alpha\beta} \left[\Lambda_f^{(+)} \right]_{\beta\alpha}$$

$$= \frac{1}{2} \left[H' \Lambda_i^{(+)} \gamma_4 H'^{\dagger} \gamma_4 \Lambda_f^{(+)} \right]_{\alpha\beta}$$

$$= \frac{1}{2} T_r \left(H' \Lambda_i^{(+)} \gamma_4 H'^{\dagger} \gamma_4 \Lambda_f^{(+)} \right)$$
...(226)

Thus the problem of finding the transition probability is reduced to the evaluation of a trace in which the explicit form of the free particle spinors is not needed.

Motivated by it we now try to construct the projection operators for the states of specified spins, so that we may compute the transition probability between states with particular values of helicity (projection of spin in the direction of the motion); without any recourse to the explicit form of the helicity eigenfunctions.

In the Pauli spin formalism, it is well known that

$$\frac{1+\sigma \cdot \hat{n}}{2} \qquad \dots (227)$$

is the projection operator for a two-component spinor whose spin direction is \hat{n} .

To find the analogous operators for the four component spinors in the relativistic theory, we go to the rest frame (see prob. 5), where the spin is most easily described, and try to find a projection operator which may be cast into a covariant form. Guided by eqn. (227), we may try

$$\frac{1+\overrightarrow{\sigma'}\cdot \widehat{n}}{2} \qquad \dots (228)$$

However, as we can at once verify from eqn. (70) a free-particle spinor is, in general, not an eigenspinor of $\sigma' \cdot n$. Moreover, this form is not manifestly covariant. Therefore noting that σ'_k and $\beta \sigma'_k = -i\gamma_5 \gamma_k$ have the same non-relativistic limit, we may try instead

$$\Sigma (w) = \frac{1 - i \gamma_5 \gamma. w}{2} \dots (229)$$

where w_n is a four-vector such that for the electron in the rest frame it is a unit (three) vector with a vanishing fourth component; i.e.,

$$|w_{\mu}|_{\text{rest frame}} = (\hat{n}, 0)$$
 ...(230)

The physical meaning of w_{μ} is such that when we consider a Lorentz transformation which brings the electron to rest, then in that rest frame, (229) is the projection operator for electron spin state whose spin points in the direction \hat{n} . For general spin vector S_{μ} , with $S_{\mu}p_{\mu}=0$,

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...(231)

$$\Sigma(s) = \frac{1 - i\gamma_5 \gamma \cdot s}{2}.$$

Thus in the rest frame, $\Sigma (w_z) u^1 = \frac{1 - i\gamma_5 \gamma_z}{2} u^1 = \frac{1 + \beta_5'}{2} u^1 = u^1,$

and $\Sigma (-w_2) u^2 = \frac{1+i\gamma_5\gamma_2}{2} u^2 = \frac{1-\beta_5'}{2} u^2 = u^2$.

Similarly, for the negative energy spinors Σ $(-w_z)$ $v^1 = v^1$ and Σ (w_z) $v^2 = v^2$

Because of the covariant form of the projection operator $\Sigma(s)$, for any polarization vector $S_{\mu}(S_{\mu}p_{\mu}=0)$, we may write Σ (s) $u^{1}(\uparrow) = u^{1}(\uparrow)$

 Σ (s) $v^{1}(\uparrow) = v^{1}(\uparrow)$ $\Sigma (-s) u^{1} (\uparrow) = \Sigma (-s) v^{1} (\uparrow) = 0$

With the four projection operators $\bigwedge^{(\pm)}(p)$ and $\Sigma(\pm s)$ we can completely specify the free-particle motion in terms of p_{μ} , sign of energy E_p , and polarization S_{μ} with $S_{\mu} p_{\mu} = 0$. We can use these projection operators to develop rapid and efficient computational techniques. They permit us to use closure methods thus avoiding the necessity of writing out matrices and spinor. solutions, component by component.

10.15. BILINEAR COVARIANTS:

Quantities of the form $\bar{\psi}\Gamma\psi$, where Γ is a product of gamma matrices, are known as Bilinear covariants or Dirac invariants; because they have definite transformation properties under Lorentz transformations, as will be seen in a moment. To list all possible bilinear covariants, let us start multiplying the gamma matrices.

If we multiply any pair of gamma matrices, we get either $\gamma_{\mu}^2=1$, when the two matrices are the same; or $\gamma_{\mu}\gamma_{\nu}=-\gamma_{\nu}\gamma_{\mu}=i\sigma_{\mu\nu}$, when the two matrices are different.

When we multiply three gamma matrices, we get back to one of the γ_{μ} 's up to a sign, unless all the three matrices are different (for example $\gamma_3\gamma_2\gamma_3 = -\gamma_3\gamma_3\gamma_3 = -\gamma_2$). When all the three matrices are different, we do get a new matrix $\gamma_{\mu}\gamma_{\nu}\gamma_{\lambda}$. But $\gamma_{\mu}\gamma_{\nu}\gamma_{\lambda}$, with $\mu \neq \nu \neq \lambda$, can always be written in the form $\gamma_5 \gamma_\rho$ up to a sign, where $\rho \neq \mu$, ν , λ (for example,

 $\gamma_3\gamma_2\gamma_4=\gamma_1\gamma_1\gamma_3\gamma_2\gamma_4=-\gamma_1\gamma_1\gamma_2\gamma_3\gamma_4=-\gamma_1\gamma_5=\gamma_5\gamma_1).$ Finally, when we multiply four gamma matrices, we get only one new matrix $\gamma_5 = \gamma_1 \gamma_2 \gamma_3 \gamma_4$ (which, of course, is equal to $-\gamma_2\gamma_3\gamma_4\gamma_1$, $\gamma_3\gamma_4\gamma_1\gamma_2$, etc.)

Needless to say, when we multiply five or more gamma matrices, we obtain nothing new. Therefore,

$$\Gamma_A=1, \gamma_\mu, \sigma_{\mu\nu}=-i\gamma_\mu\gamma_\nu \ (\mu\neq\nu), i\gamma_5\gamma_\mu \ \text{and} \ \gamma_5 \dots (232)$$

represent all possible combinations. These are 16 independent matrices: the identity matrix, four γ_{μ} matrices, six $\sigma_{\mu\nu}$ matrices, four $i\gamma_5\gamma_{\mu}$ matrices, and the γ_5 matrix. The factors $\pm i$ in (232) are inserted to get,

$$F_A^2=1$$
; $A=1, 2, \dots, 16$...(233)

Thus we can have the following five types of bilinear covariants: $S = \bar{\psi}\psi$, $V_{\mu} = \bar{\psi}\gamma_{\mu}\psi$, $T_{\mu\nu} = \bar{\psi}\sigma_{\mu\nu}\psi$, $A_{\mu} = i\bar{\psi}\gamma_{5}\gamma_{\mu}\psi$ and $P = \bar{\psi}\gamma_{5}\psi$...(234) Now we investigate the behaviour of these bilinear covariants under Lorentz transformations. Under proper Lorentz transformation $\psi'(x') = S\psi(x)$ (note that this S is different than the $S = \bar{\psi}\psi$) we have,

$$S' = \overline{\psi}'\psi' = \psi^{\dagger}S^{\dagger}\gamma_{4}S\psi = \psi^{\dagger}\gamma_{4}\gamma_{4}S^{\dagger}\gamma_{4}S\psi$$

$$= \psi^{\dagger}\gamma_{4}S^{-1}S\psi \qquad \{ : \gamma_{4}S^{\dagger}\gamma_{4} = S^{-1} \}$$

$$= \overline{\psi}\psi = S$$

For the behaviour under space inversion, we obtain

$$S' = \overline{\psi}'\psi' = e^{-i\xi}\overline{\psi}\gamma_4.e^{i\xi}\gamma_4\psi = \overline{\psi}\psi = S$$

Thus we find that S is invarient under proper Lorentz transformation and the space inversion; hence it is a scalar.

To investigate the transformation properties of V_{μ} we have,

$$V_{\mu}' = \overline{\psi}' \gamma_{\mu} \psi' = \overline{\psi}(x) S^{-1} \gamma_{\mu} S \psi(x) = a_{\mu} \psi \gamma_{\nu} \psi = a_{\mu\nu} V_{\nu},$$

under homogeneous proper Lorentz transformation. For the behaviour under space inversion, we obtain

$$V_{\mu}' = \overline{\psi}' \gamma_{\mu} \psi' = e^{-i\xi} \overline{\psi} \gamma_{4} \gamma_{\mu} e^{i\xi} \gamma_{4} \psi$$

$$= \overline{\psi} \gamma_{4} \gamma_{\mu} \gamma_{4} \psi \Rightarrow$$

$$V_{i}' = \overline{\psi} \gamma_{4} \gamma_{i} \gamma_{4} \psi$$

$$= -\overline{\psi} \gamma_{4} \gamma_{i} \gamma_{4} \psi = -\overline{\psi} \gamma_{i} \psi = -V_{i} \ (i=1, 2, 3),$$

$$V_{A}' = \overline{\psi} \gamma_{4} \gamma_{4} \gamma_{4} \psi = \overline{\psi} \gamma_{4} \psi = V_{4}$$

and

Hence V_{μ} is a four-vector whose space components change under parity.

Using similar techniques we find that $T_{\mu\nu} = \bar{\psi}\sigma_{\mu\nu}\psi = -i\bar{\psi}\gamma_{\mu}\gamma_{\nu}\psi$ with $\mu \neq \nu$ (which is necessarily antisymmetric in μ and ν) is a second rank tensor.

Also we have under space inversion,

$$A_{\mu}' = i\bar{\psi}'\gamma_5\gamma_{\mu}\psi' = i\bar{\psi}\gamma_4\gamma_5\gamma_{\mu}\gamma_4\psi$$

or

and
$$\begin{aligned} \therefore & A_{i}' = i\overline{\psi}\gamma_{4}\gamma_{5}\gamma_{i}\gamma_{4}\psi = -i\overline{\psi}\gamma_{5}\gamma_{4}\gamma_{1}\gamma_{4}\psi \\ &= i\overline{\psi}\gamma_{5}\gamma_{i}\gamma_{4}\gamma_{4}\psi = i\overline{\psi}\gamma_{5}\gamma_{i}\psi = A_{i} \ (i=1,\,2,\,3), \\ A_{4}' = i\overline{\psi}\gamma_{4}\gamma_{5}\gamma_{4}\gamma_{4}\psi = i\overline{\psi}\gamma_{4}\gamma_{5}\psi \\ &= -i\overline{\psi}\gamma_{5}\gamma_{4}\psi = -A_{4} \end{aligned}$$

Whereas under proper Lorentz transformation it can be seen to transform in the same way as V_{μ} . Thus A_{μ} behaves like an axial vector (pseudovector).

Finally, using similar arguments, we can easily see that P transforms exactly like the scalar S under proper homogeneous Lorentz transformation but changes its sign under space inversion. It is the characteristic of a pseudoscalar. We summarize the results in the following table:

Quantity	Proper homogeneous Lorentz transformation	Space
Scalar, $S = \overline{\psi} \psi$	$\bar{\psi}\psi$	$\bar{\psi}\psi$
Vector, $V_{\mu} = \overline{\psi} \gamma_{\mu} \psi$	のよりサンツ	$\begin{bmatrix} -\overline{\psi}\gamma_i\psi \\ \overline{\psi}\gamma_4\psi \end{bmatrix},$
Tensor $T_{\mu\nu} = \overline{\psi} \sigma_{\mu\nu} \psi$ (antisymmetric)	σμλαυρψολρψ	$\begin{bmatrix} \bar{\psi}_{\sigma_{i:i}} i \\ -\bar{\psi}_{\sigma_{i:i}} \psi \end{bmatrix}$
Axial vector $A_{\mu} = i \bar{\psi} \gamma_5 \gamma_{\mu} \psi$ (pseudovector)	$a_{,\nu}i\bar{\psi}\gamma_{5}\gamma_{\nu}\psi$	$\begin{bmatrix} i\bar{\psi}\gamma_5\gamma_4\psi \\ -i\bar{\psi}\gamma_5\gamma_4\psi \end{bmatrix}$
Pseudoscalar $P = \Psi \gamma_5 \psi$	$\psi_{\gamma_5}\psi$	$-\bar{\psi}\gamma_{5}\psi$

10.16. ZERO MASS DIRAC EQUATION:

Particles with zero mass and spin $\frac{1}{2}$ are, indeed, found in nature; they are the neutrinos. For such particles, the Dirac Hamiltonian will not involve β , and the Hamiltonian form of the Dirac equation becomes:

$$i \frac{\partial \chi(x)}{\partial t} = -i \stackrel{\rightarrow}{\alpha} \cdot \nabla \chi(x) = i \stackrel{\rightarrow}{\gamma} \cdot p_{\chi}(x)$$

$$i \frac{\partial \chi(x)}{\partial t} = i \stackrel{\rightarrow}{\gamma} \cdot p_{\chi}(x)$$
...(235)

We define the 'helicity operator' as $h(p) = \frac{\sigma' \cdot p}{|p|}$, which gives the projection of spin in the direction of motion. (Through the

spin is not a constant of motion for Dirac particle but helicity is a constant of motion) Since σ' can be expressed as $\sigma' = -i\gamma_5\gamma_4\gamma$, we can write the Hamiltonian as:

$$H = i\gamma_{4}\gamma \cdot \mathbf{p} = i\gamma_{5}\gamma_{5}\gamma \cdot \mathbf{p} = -\gamma_{5}\sigma' \cdot \mathbf{p}$$

$$= -\gamma_{5} \mid \mathbf{p} \mid h(\mathbf{p}) \qquad ...(236)$$

The eigenfunctions of H and h(p) are, therefore, also the eigenfunctions of γ_5 .

Since the zero mass equation does not contain the β matrix, and the anticommutation relations for the three matrice α_1 , α_2 and α_3 may be satisfied with the 2×2 Pauli matrices σ_1 , σ_2 and σ_3 zero mass particle can be described by two component equation

$$i \frac{\partial \varphi(x)}{\partial t} = \stackrel{\rightarrow}{\sigma} \cdot \mathbf{p} \, \varphi(x) \qquad \dots (237)$$

The possibility of describing massless Dirac particles by a two component equation was first discussed by Weyl but was not taken seriously, the reason being that the $\beta \equiv \gamma_4$ matrix, and thus the parity operation $P = e^{i\xi}\gamma_4$, has been lost in reducing to two components. After the violation of parity in 1956, Lee and Yang resurrected the Weyl's equation. They also observed that the zero mass equation lost the charge conjugation symmetry,

$$C \sim \gamma_4 \gamma_2$$

due to γ_4 for which there is no place in the equation. However, it is invariant under the combined transformation

$$CP \sim \gamma_2 = \sigma_2$$

Problems

Problem 1. Find an expression for the current of a K.G. particle in the presence of an electromagnetic field A_{+} .

Sol. The K.G. equation $(\Box - m^2) \phi = 0$ for a free particle can be written as:

$$\partial_{\mu}^{2}\phi - m^{2}\phi = 0 \qquad \dots (i)$$

The interaction with field can be introduced by replacing ∂_{μ} by $(\partial_{\mu} - ieA_{\mu})$. Therefore, in the presence of the e.m. field A_{μ} , K.G. equation can be written as:

$$(\hat{\partial}_{\mu} - ieA_{\mu})^2 \phi - m^2 \phi = 0 \qquad ...(ii)$$

Taking its complex conjugate, we obtain

$$\phi^* (\partial_{\mu} + ieA_{\mu})^2 - m^2 \phi^* = 0$$
 ...(iii)

Multiplying (ii) from left by ψ^* and (iii) from the right by ϕ and subtracting one form the other we get:

and subtractive
$$\phi^{*}(\partial_{\mu}^{2}\phi) - (\partial_{\mu}^{2}\phi^{*}) \phi - 2ie\phi^{*}A_{\mu}(\partial_{\mu}\phi) - 2ie(\partial_{\mu}\phi^{*}) A_{\mu}\phi = 0$$

$$\phi^{*}(\partial_{\mu}^{2}\phi) - (\partial_{\mu}^{2}\phi^{*}) \phi - 2ie\phi^{*}A_{\mu}(\partial_{\mu}\phi) - 2ie(\partial_{\mu}\phi^{*}) A_{\mu}\phi = 0$$

$$(\partial_{\mu} - ieA_{\mu})^{2} = (\partial_{\mu} - ieA_{\mu}) (\partial_{\mu} - ieA_{\mu})$$

$$= \partial_{\mu}^{2} - ie A_{\mu}\partial_{\mu} - ie\partial_{\mu} A_{\mu} - e^{2}A_{\mu}^{2}$$

$$= \partial_{\mu}^{2} - 2ie A_{\mu}\partial_{\mu} - e^{2}A_{\mu}^{2} \text{ as } [\partial_{\mu}, A_{\mu}] = 0$$

$$\Rightarrow \qquad (\partial_{\mu} - ieA_{\mu}) - (\partial_{\mu}\phi^{*}) A_{\mu}\phi = 0$$

$$= \partial_{\mu}^{2} - 2ie A_{\mu}\partial_{\mu} - e^{2}A_{\mu}^{2} \text{ as } [\partial_{\mu}, A_{\mu}] = 0$$

 $\partial_{\mu} \left[\phi^{*}\partial_{\mu}\phi^{*}\partial_{\mu}\phi\right] - \partial_{\mu} \left[2ie\phi^{*}A_{\mu}\phi\right] = 0$

or

Defining $\phi^*\partial_{\mu}\phi = \frac{1}{2} [\phi^*\partial_{\mu}\phi - \phi^*\partial_{\mu}\psi]$, we get

$$\partial_{\mu} \left[2\phi^{*}\partial_{\mu}\phi - 2ie\phi^{*}A_{\mu}\phi\right] = 0 \qquad ...(iv)$$

Comparing it with the equation of continuity $\partial_{\mu} j_{\mu} = 0$ we find the expression for the current as:

$$j_{\mu} = 2\phi^* \partial_{\mu} \psi - 2ie\phi^* A_{\mu} \phi \qquad ... (v)$$

More explicitly, we can write (v) as:

$$j_{\mu} = \phi^* \left(\overrightarrow{\partial}_{\mu} - ieA_{\mu} \right) \phi - \phi^* \left(\overrightarrow{\partial}_{\mu} + ieA_{\mu} \right) \phi \qquad ...(vi)$$

Problem 2. Show that the K. G. equation can be put into the form of Schroedinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \qquad ...(i)$$

where ψ is a two component wavefunction and H is the K.G. Hamiltonian.

Sol. Introducing two component wavefunction,

$$\psi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix},$$

the K. G. equation $\left(\frac{-p^2}{\hbar^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \psi = \frac{m^2 c^2}{\hbar^2} \psi$ is equivalent to the following two equations:

$$\left(-\frac{p^2}{\hbar^2} - \frac{1}{c^2} \int_{0}^{2} \frac{\partial^2}{\partial t^2}\right) \varphi_1 = \frac{m^2 c^2}{\hbar^2} \varphi_3 \qquad \dots \text{(iia)}$$

and

$$\left(-\frac{p^2}{\hbar^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \varphi_2 = \frac{m^3 c^2}{\hbar^2} \varphi_2. \qquad \dots \text{(iib)}$$

If we define a Hamiltonian $H=(\sigma_z+i\sigma_y)\frac{\vec{p}^2}{2m}+mc^2\sigma_z$, then we can show that the equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

is equaivalent to the K. G. equations (ii). (σ_y and σ_z in the above are the Pauli-spin matrices). We have

the Pauli-spin matrices). We have
$$i\hbar \frac{\partial}{\partial t} \binom{\varphi_1}{\varphi_2} = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + i \begin{pmatrix} 0 & -i \\ i & 0 \end{bmatrix} \right\} \frac{p^2}{2m} + mc^2 \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix} \right\} \binom{\varphi_1}{\varphi_2}$$

$$\Rightarrow i\hbar \frac{\partial \varphi_1}{\partial t} = \left(\frac{p^2}{2m} + mc^2 \right) \varphi_1 + \frac{p^2}{2m} \varphi_2 \qquad ...(iiia)$$

and

$$i\hbar\frac{\partial\varphi_2}{\partial t} = -\frac{p^2}{2m}\varphi_1 - \left(\frac{p^2}{2m} + mc^2\right)\varphi_2.$$
 ... (iiib)

Putting the value of φ_1 from (iii b) into (iii a), and making a little simplification we get

$$\left(-\frac{p^2}{\hbar^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \varphi_2 = \frac{m^2 c^2}{\hbar^2} \varphi_2 \qquad ...(iv)$$

Similarly, putting the value of φ_2 from (iii a) into (iii b) and simplifying, we get

$$\left(-\frac{p^2}{\hbar^2} - \frac{1}{c^2} \frac{\tilde{c}^2}{\partial t^2}\right) \varphi_1 = \frac{m^2 c^2}{\hbar^2} \varphi_2. \qquad \dots (v)$$

From (iv) and (v), we see that with

$$H = (\sigma_z + i\sigma_y) \frac{p^2}{2m} + mc^2 \sigma_z,$$

we can write the K. G. equation in the form of Schroedinger equation (i).

Problem 3. Find the Schroedingar form of the Dirac equation

for a charged particle in an e. m field Au.

Sol. The Dirac equation for a particle of charge -e, in the presence of the e.m. field $A_{\mu} = (A, iA_0)$ can be written as

$$\begin{bmatrix} \overrightarrow{\gamma} & \left(p - \frac{e}{c} \overrightarrow{A} \right) + \gamma_4 & \left(\frac{-i\hbar}{ic} \frac{\partial}{\partial t} + \frac{e}{ic} A_0 \right) - imc \end{bmatrix} \psi = 0$$

Multiplying it on the left by icy4, we obtain the Dirac equation in "Schroedinger" form

if
$$\frac{\partial \psi}{\partial t} = \begin{bmatrix} \overrightarrow{c} & \overrightarrow{\alpha} & (\mathbf{p} - \frac{e}{c} \mathbf{A}) + mc^2\beta + cA_0 \end{bmatrix} \psi$$
. ...(i)

Problem. 4. Find the time dependence of the position operator r of a free particle of spin $\frac{1}{2}$ in the Heisenberg picture. Discuss the result obtained.

Sol. The positive and the negative energy plane wave soluson of the Dirac equation are given by

$$\psi_{E > 0} = \frac{1}{\sqrt{(V)}} u^{r} \text{ (p) exp. } [i \text{ (p.r-}E_{p}t)/\hbar] \\
\psi_{E < 0} = \frac{1}{\sqrt{(V)}} v^{r} \text{ (p) exp. } [i \text{ (p.r+}E_{p}t)/\hbar]. \\$$
...(i)

Since the solutions (i) with all possible p form a complete orthonormal set, the most general free particle wave function can be written as

$$\psi(\mathbf{r},t) = \sum_{p} \sum_{r=1}^{2} \sqrt{\left(\frac{mc^{2}}{E_{p}V}\right)} c_{p}, \quad u^{r}(\mathbf{p}) \exp \left[i\left(\mathbf{p}.\mathbf{r} - E_{p}t\right)/\hbar\right]$$

$$+ \sum_{p} \sum_{r=1}^{2} \sqrt{\left(\frac{mc^{2}}{E_{p}V}\right)} d_{p}, \quad v^{r}(\mathbf{p}) \exp \left[i\left(\mathbf{p}.\mathbf{r} + E_{p}t\right)/\hbar\right],$$
...(ii)

where the expansion coefficient c_p , r and d_p , r can be determined from the Fourier expansion of ψ at t=0. Let us now evaluate the expectation value of the matrix α . We have

expectation value of the matrix
$$\vec{\alpha}$$
. We have
$$\vec{\langle \alpha \rangle} = \int \psi^{\dagger}(\mathbf{r}, t) \vec{\alpha} \psi(\mathbf{r}, t) d^{3}r$$

$$= \sum_{p,p'} \sum_{r,r'=1}^{2} \sqrt{\left\{\frac{(mc^{2})^{2}}{E_{p}E_{p'}V^{2}}\right\}} c_{p',r'}^{*}, c_{p,r} u^{r'\dagger}(\mathbf{p}) \vec{\alpha} u^{r'}(\mathbf{p}) V \delta_{p,p'}$$

$$= \sum_{p,p'} \sum_{r,r'=1}^{2} \sqrt{\left\{\frac{mc^{2})^{2}}{E_{p}E_{p'}V^{2}}\right\}} d_{p'r'}^{*}, d_{p,r} v^{r'\dagger}(\mathbf{p}) \vec{\alpha} v^{r}(\mathbf{p}) V \delta_{p,p'}$$

$$= \sum_{p,p'} \sum_{r,r'=1}^{2} \frac{mc^{2}}{E_{p}} \left\{d_{p,r'}^{*}c_{p,r} v^{r'\dagger}(\mathbf{p}) \vec{\alpha} u^{r}(\mathbf{p}) e^{-2iE_{p}t/\hbar}\right\}$$

$$= \sum_{p} \sum_{r=1}^{2} |c_{p,r}|^{2} \frac{pc}{E_{p}} - \sum_{p} \sum_{r=1}^{2} |d_{p,r}|^{2} \frac{pc}{E_{p}}$$

$$+ \sum_{p} \sum_{r'=1}^{2} \frac{mc^{2}}{E_{p}} \left\{d_{p,r'}^{*}c_{p,r} v^{r'\dagger}(\mathbf{p}) \vec{\alpha} u^{r}(\mathbf{p}) e^{-2iE_{p}t/\hbar}\right\}$$

$$+ \sum_{p} \sum_{r'=1}^{2} \frac{mc^{2}}{E_{p}} \left\{d_{p,r'}^{*}c_{p,r} v^{r'\dagger}(\mathbf{p}) \vec{\alpha} v^{r}(\mathbf{p}) e^{2iE_{p}t/\hbar}\right\} ...(iii)$$

As for $\langle \mathbf{r} \rangle$, we first observe that the operator relation $\dot{\mathbf{r}} = c\alpha$ implies that

 $\frac{d}{dt} \int \psi_1^* (\mathbf{r}, t) \mathbf{r} \psi (\mathbf{r}, t) d^3 r = c \int \psi_1^* (\mathbf{r}, t) \overset{\Rightarrow}{\alpha} \psi (\mathbf{r}, t) d^3 r. \dots (iv)$

We can, therefore, obtain $\langle r \rangle$ by integrating c times (iii) with respect to 't':

$$\langle \mathbf{r} \rangle = \langle \mathbf{r} \rangle_{t=0} + \sum_{p} \sum_{r=1}^{2} |c_{p}, r|^{2} \frac{\mathbf{p}c}{E_{p}} t - \sum_{p} \sum_{r=1}^{2} |d_{p}, r|^{2} \frac{\mathbf{p}c}{E_{p}} t$$

$$+ \sum_{p} \sum_{r'=1}^{2} \frac{i\hbar}{2mc} \left(\frac{mc^{3}}{E_{p}}\right)^{2} \left\{ d_{p}^{*}, r'c_{p}, r'^{\dagger}(\mathbf{p})\overset{\rightarrow}{\alpha} u^{*}(\mathbf{p}) e^{-2iE_{p}t/\hbar} - d_{p}, r'c_{p}, r''(\mathbf{p})\overset{\rightarrow}{\alpha} v''(\mathbf{p}) e^{2iE_{pt}/\hbar} \right\}. \qquad (v)$$

Expression (v) represents the time dependence of the position operator in the Heisenberg picture. From it, the motion of the centroid (r) of a wave-packet for a free particle with spin ½ can be found. The first (second) term which is time independent represents the motion of the wave-packet made up exclusively of positive (negative) energy plane wave components. The last two terms,

which are time dependent, are more interesting. α taken between v^{\dagger} and u is "large" when $|\mathbf{p}| < mc$, in sharp contrast with α taken between u^{\dagger} and u which is of order v/c. Therefore, last two terms of (v) represent a superposition of violent and rapid oscillations, each with an angular frequency $\sim 2mc^2/\hbar$. Thus we see that, in addition to the classical uniform motion in a straight line, the centroid of the wave-packet has a rapid oscillatory motion whose amplitude and period are of the order of \hbar/mc and \hbar/mc^2 , respectively. This oscillatory motion was called the 'Zitterbewgung' by Schroedinger. It should be noted that this peculiar oscillatory behaviour of $\langle \mathbf{r} \rangle$ is due to an interference between the positive and negative energy components in the wave-packet. The Zitterbewgung is completely absent for a wave-packet made up exclusively of +ve (--ive) energy plane wave solutions.

Due to Zitterbewgung, the localization of a free particle is possible only in a volume of linear dimension of order \hbar/mc . It

imparts the value $\pm c$ to the velocity of the electron. However, the imparts is so high that in actual measurements the imparts the value of that in actual measurements the departure frequency is not observed. Zitterbewgung do not appearance it is done to be a process of the departure frequency is not observed. Zitterbewgung do not appear in nonfrom c^2p/E_p is not observed it is due to the rest mass from c²p/Ep 13 heary because it is due to the rest mass energy of the relativistic.

problem 5. Show that for a positive energy spinor $u(p) = \overline{A} (m-i\gamma_{-n}) u(0)$ particle. $u(\mathbf{p}) = \overline{A}(m-i\gamma \cdot p) u(0)$...(i)

and find the normalization constant A. The equation (i) gives a relationship between the spinor with momentum p to the spinor in the rest frame. As we pointed with momentum is most easily described in the with monitor, the spin is most easily described in the zero momen-out earlier, the spin is most easily described in the zero momenout earner, and hence we are interested in finding out a transtum trains of the type (i). In order to get (i), we have the Lorenformation to the rest frame as tez transformation to the rest frame as

 $u(p) = \exp \left[\frac{1}{4} a_{\mu\nu} \sigma_{\mu\nu}\right] u(0) \equiv (A + B\gamma \cdot p) u(0).$...(ii)

Multiplying both sides of (ii) by $(i\gamma.p+m)$ and using the Dirac equation (iy. p+m) u(p)=0, we obtain

$$i\gamma. pA + mA + m\gamma. pB + ip^2B = 0$$

 $i\gamma. pA + mA + m\gamma. pB - im^2B = 0$
 $i\gamma. pA + mA + m\gamma. pB - im^2B = 0$
 $p^2 = -m^2$

Clearly, (iii) is satisfied for mB = -iA. Hence we can write

(ii) as $u(p) = \bar{A}(m-i\gamma.p) u(0),$

where $\overline{A} = \frac{A}{m}$ is a new constant.

· or

To find the normalization constant A, we have the condition u u=1. Now

$$\overline{u}(p) = u\dagger(p) \gamma_4 = \overline{A^*} \underbrace{u\dagger(0) (m-i \gamma. p)\dagger \gamma_4}_{=\overline{A^*}}$$

$$= \overline{A^*} \underbrace{u(0) (m-i \gamma. p)\dagger \gamma_4}_{=\overline{A^*}}$$

$$= \overline{A^*} \underbrace{u(0) (m-i \gamma. p)}_{=\overline{A^*}}.$$

Thus, we get

$$u(p) = \frac{m-i \gamma \cdot p}{\sqrt{[2m (m+E_p)]}} u(0).$$
 ...(iv)

Problem 6. Show that for a Dirac particle in the presence of a central potential V(r), following quantities are constants of motion:

(a) S^2 , (b) J and (c) K.

Sol. The Hamiltonian for a Dirac particle in the presence of the potential V(r) is written as:

$$H = c \stackrel{\rightarrow}{\alpha} p + \beta mc^2 + V(r) \qquad ...(i)$$
Now, $[S^2, H] = [S_x^2, H] + [S_y^2, H] + [S_z^2, H] \qquad ...(ii)$

$$[S_x^2, H] = S_x [S_x, H] + [S_x, H] S_x$$
 ...(iii)

We have

$$S_x = \frac{1}{2} \hbar \sigma_x' = \frac{1}{2} \hbar \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} = \frac{1}{2} \hbar \alpha_x \rho_1$$
, where $\rho_1 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$

Thus we have:

$$[S_x, H] = \frac{1}{2} \, \ln c \rho_1 \quad \{\alpha_x \left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z\right) - \left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z\right) \alpha_x\}$$

$$\{ :: \alpha_x \text{ commutes with } \beta \text{ and } V(r) \}$$

$$= \frac{1}{2} \, \ln c \rho_1 \quad \{\alpha_x \alpha_y p_y + \alpha_x \alpha_z p_z - \alpha_y \alpha_x p_y - \alpha_z \beta_x p_z\}$$

$$= \ln c \rho_1 \quad \{\alpha_x \alpha_y p_y + \alpha_x \alpha_z p_z\} \quad [\text{Using } \alpha_x \alpha_y = -\alpha_y \alpha_x \text{ etc.}]$$

$$\therefore \quad S_x \left[S_x, H \right] = \frac{1}{2} \, \ln^2 c \quad \{\alpha_x \alpha_x \alpha_y p_y + \alpha_x \alpha_x \alpha_z p_z\} \quad [\text{:: } \rho_1^2 = 1]$$

$$= \frac{1}{2} \, \ln^2 c \quad \{\alpha_y p_y + \alpha_z p_z\} \quad [\text{:: } \alpha_x^2 = 1]$$

$$[S_x, H] \quad S_x = \frac{1}{2} \, \ln^2 c \quad \{\alpha_y \alpha_y \alpha_x p_y + \alpha_x \alpha_z \alpha_z p_z\}$$

$$= \frac{1}{2} \, \ln^2 c \quad \{-\alpha_x \alpha_x \alpha_y p_y - \alpha_x \alpha_x \alpha_z p_z\}$$

$$= -\frac{1}{2} \, \ln^2 c \quad \{\alpha_y p_y + \alpha_z p_z\}$$

and

Hence we have:

$$[S_x^2, H] = S_x [S_x, H] + [S_x, H] S_x = 0.$$

Similarly we can show that:

$$[S_v^2, H] = [S_z^2, H] = 0$$

and this implies that

 $[S^2, H] = [S_x^2, H] + [S_y^2, H] + [S_z^2, H] = 0$. Therefore, S^2 is a constant of motion.

To show that J is a constant of motion, we have from the article 10.6:

$$J=L+\frac{1}{2}\hbar \sigma', \text{ and}$$

$$[L_x, H]=-i\hbar c (\alpha_z p_y - \alpha_y p_z);$$

$$[\sigma_x', H]=2ic (\alpha_z p_y - \alpha_y p_z)$$

$$\therefore [J_x, H]=[L_x+\frac{1}{2}\hbar\sigma_x', H]$$

$$=[L_x, H]+\frac{1}{2}\hbar [\sigma_x', H]=0$$

Similarly, we can show that

$$[J_y, H] = [J_z, H] = 0$$

Hence J is a constant of motion.

Lastly, for $K=\beta$ (σ' .L+ \hbar) we have:

$$[K, H] = c [\beta \overrightarrow{\sigma}'.L, \alpha.p] + 2\beta c \hbar (\alpha p)$$

{: β and V(r) commutes with K}

Now,

$$[\beta \overrightarrow{\sigma}'. L, \overrightarrow{\alpha}.p] = \beta (\overrightarrow{\sigma}', L) (\overrightarrow{\alpha}.p) - (\overrightarrow{\alpha}.p) \beta (\overrightarrow{\sigma}', L)$$

$$= \beta (\overrightarrow{\sigma}'.L)(\overrightarrow{\alpha}.p) + \beta (\overrightarrow{\alpha}.p)(\overrightarrow{\sigma}'.L) \qquad ...(iv)$$

Using the explicit form of the matrices σ' , α and γ_5 , we can show that for any operators A and B which commute with σ ,

$$(\alpha.A)(\sigma'.B) = -\gamma_5 (A.B) + i \alpha. (A \times B)$$
 ...(v)

and

$$(\sigma'.A)(\alpha.B) = -\gamma_5 \quad (A.B) + i \quad \alpha \quad (A \times B)$$
 ...(vi)

Using (v) and (vi) we can write (iv) as:

$$[\beta \overrightarrow{\sigma'}. L, \overrightarrow{\alpha}.p] = \beta[-\gamma_5 (L.p) + i \overrightarrow{\alpha}. (L\times p) - \gamma_5 (p.L) + i \overrightarrow{\alpha} (p\times L)]$$

Now
$$\mathbf{p}.\mathbf{L} = \mathbf{p}.((\mathbf{r} \times \mathbf{p}) = 0 \text{ and } \mathbf{L}.\mathbf{p}. = (r \times \mathbf{p}).\mathbf{p} = 0$$
 ...(vii)

Also,

$$L \times p + p \times L = -r p^2 + (r.p) p + rp^2 - (p \cdot r) p + i\hbar p$$

$$= 2i\hbar p \quad \{ : (r.p - p.r) p = [r, p] = i\hbar p \}$$

 $\therefore [\beta \overrightarrow{\sigma'}.L, \overrightarrow{\alpha}.p] = -2\hbar\beta \overrightarrow{\alpha}p$

and hence we have

$$[K, H] = -2\beta \hbar c (\alpha.p) + 2\beta \hbar c (\alpha.p) = 0$$

Thus K commutes with H and hence it is a constant of motion.

Problem 7. For a free particle Dirac hamiltonian, $H = \alpha . \mathbf{p} + m\beta$, obtain a unitary transformation which will eliminate the 'odd' operator α . Discuss briefly the physical significance of this transformation.

Sol. Let the required transformation be carried out by the unitary operator $U=e^{iS}$ where S is hermitian and not explicitly time dependent. Then the transformed wavefunction and the transformed Hamiltonian are given; respectively, by

$$\psi' = e^{iS} \psi
H' = e^{iS} He^{-iS}$$

and

H' is to contain no odd operators by construction.

Since $H=\alpha.p+\beta m$, with $[\alpha, \beta]=0$, our problem is quite analogous to that of attempting to find a unitary transformation which changes a two component spin Hamiltonian

 $H = A_1 \sigma_1 + A_3 \sigma_3 \qquad \cdots (ii)$

into a form which contains only even operators. Such a transformation is simply a rotation about y-axis and the operator is exp. $\left(\frac{i}{2} \sigma_2 \theta\right)$. The transformed Hamiltonian will be given by:

$$H' = \exp\left\{\frac{i}{2} \cdot \sigma_{2}\theta\right\} + \exp\left\{-\frac{i}{2} \cdot \sigma_{2}\theta\right\}$$

$$= \left(\cos\frac{\theta}{2} + i\sigma_{2}\sin\frac{\theta}{2}\right) (A_{1}\sigma_{1} + A_{3}\sigma_{3}) \left(\cos\frac{\theta}{2} - i\sigma_{2}\sin\frac{\theta}{2}\right)$$

$$= A_{1}\sigma_{1}\cos\theta + A_{3}\sigma_{3}\cos\theta + 2\sigma_{3}A_{1}\sin\theta - \sigma_{1}A_{3}\sin\theta$$

$$\{: \sigma_{2}\sigma_{1}\sigma_{2} = -\sigma_{1}; \sigma_{2}\sigma_{3}\sigma_{2} = -\sigma_{3} \text{ and } \sigma_{1}\sigma_{2} = i\sigma_{3}\}$$

Since we want that H' should be free from the odd operator σ_1 , we equate its coefficient in H' equal to zero. We obtain:

 $A_1 \cos \theta - A_3 \sin \theta = 0$ $\tan \theta = A_1/A_3$

or

By taking analogy from the above transformation, it is clear that in our case a good choice will be α in place of σ_1 and β in place of σ_3 , because σ_1 and α are both "odd" and σ_3 and β are both even. Therefore we take,

$$e^{iS} = \exp \left\{ \frac{1}{2} \beta \alpha \hat{p} \theta \right\}$$
 {: $i\sigma_2 = \sigma_3 \sigma_1$ }

With this choice,

$$H' = \exp. \{\beta \alpha. \hat{p} \frac{1}{2}\theta\} (\alpha. \hat{p} | p | + \beta m) \exp. \{-\beta \alpha. \hat{p} \frac{1}{2}\theta\}$$

$$= \left(\cos \frac{\theta}{2} + \beta \alpha. \hat{p} \sin \frac{\theta}{2}\right) (\alpha. \hat{p} | p | + \beta m) \left(\cos \frac{\theta}{2} - \beta \alpha. \hat{p} \sin \frac{\theta}{2}\right)$$

$$= \frac{\beta}{\alpha. \hat{p} | p | \cos \theta + \beta m \cos \theta + \beta | p | \sin \theta - m \alpha. \hat{p} \sin \theta}$$

As we want H' to be free from α , we set all the terms involving α in the above equation equal to zero; i.e.,

$$\alpha \cdot \hat{p} \mid \mathbf{p} \mid \cos \theta - m \stackrel{\rightarrow}{\alpha} \cdot \hat{p} \sin \theta = 0$$

$$\Rightarrow \tan \theta = \frac{|\mathbf{p}|}{m} \Rightarrow \sin \theta = \frac{|\mathbf{p}|}{\sqrt{(m^2 + |\mathbf{p}|^2)}} \text{ and } \cos \theta = \frac{m}{\sqrt{(m^2 + |\mathbf{p}|^2)}}$$

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Hence the transformed hamiltonian is given by:

$$H^{ence} = \frac{m}{m} \frac{|\mathbf{p}|}{\sqrt{(m^2 + |\mathbf{p}|^2)}} + \beta |\mathbf{p}| \frac{|\mathbf{p}|}{\sqrt{(m^2 + |\mathbf{p}|^2)}}$$

$$H' = \beta^m \frac{\sqrt{(m^2 + |\mathbf{p}|^2)}}{\sqrt{(m^2 + |\mathbf{p}|^2)}} \dots (ii)$$

$$= \beta \sqrt{(m^2 + |\mathbf{p}|^2)}$$

$$= \beta \sqrt{(m^2 + |\mathbf{p}|^$$

 $S = -\frac{i}{2} \beta \stackrel{\rightarrow}{\alpha} \cdot \hat{p} \tan^{-1} \left(\frac{|\mathbf{p}|}{m} \right),$

changes H into H' where H' is free from the 'odd' operator change of transformation, which removes the 'odd' terms

This type of transformation as 'the Fold.

This type and the Hamiltonian, is known as 'the Foldy Wouthysen transfrom the Hamiltonian, is known as 'the Foldy Wouthysen transfrom tion'.

In order to investigate the physical significance of the Foldy-Wouthuysen transformation, we know that except the negativeformation'. Wouldnuyson, the Dirac equation appears to provid a suitable energy problem, the electron. Foldy-Wouldness to provid a suitable energy provide a suitable description for the electron. Foldy-Wouthysen and Tani noticed that the essential reason why four-component spinors are necessthat the ary to describe a solution in the Dirac representation is that the

Hamiltonian contains the odd operators a which couples the negative and the positive energy solutions. The Foldy-Wouthuysen transformation changes the Hamiltonian into a form which is free from the odd operators and hence the solutions can be represented by two-component spinors. Thus the solution \u03c4 of the Dirac equation can be written in the form ...(iv)

 $\psi' = e^{iS} \psi = \psi'(+) + \psi'(-)$

in which $\psi'_{(+)}$ and $\psi'_{(-)}$ are the eigen-spinors of the Hamiltonian $H'=e^{iS}He^{-iS}$

with positive $(+E_p)$ and negative $(-E_p)$ eigenvalues, respectively. $\psi'_{(+)}$ and $\psi'_{(-)}$ have respectively the last two and the first two components of the four component spinors for positive and negative energies, respectively.

Problem 8. Verify the following

- (*i*) $\gamma_{\mu} \gamma_{\mu} = 4$
- (ii) $\gamma_{\mu} \gamma_{\nu} \gamma_{\mu} = -2\gamma_{\nu}$
- (iii) $\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\mu} = 4 \delta_{\lambda \nu}$
- (iv) $\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\rho} \gamma_{\mu} = -2\gamma_{\rho} \gamma_{\lambda} \gamma_{\nu}$
- $\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} + \gamma_{\lambda} \gamma_{\nu} \gamma_{\mu} = 2\delta_{\mu\nu} \gamma_{\lambda} 2\delta_{\lambda\mu} \gamma_{\nu} + 2\delta_{\nu\lambda} \gamma_{\mu}$. (v) Sol.
- (i) $\gamma_{\mu} \gamma_{\mu} = \gamma_1^2 + \gamma_2^2 + \gamma_3^2 + \gamma_4^2 = 4$

(ii)
$$\gamma_{\mu} \gamma_{\nu} \gamma_{\mu} = (2^{\varsigma}_{\mu\nu} - \gamma_{\nu} \gamma_{\mu}) \gamma_{\mu}$$

 $= 2\delta_{\mu\nu} \gamma_{\mu} - \gamma_{\nu} \gamma_{\mu} \gamma_{\mu}$
 $= 2\gamma_{\nu} - 4\gamma_{\nu} = -2\gamma_{\nu}$.

(iii)
$$\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\mu} = (2\delta_{\mu\nu} - \gamma_{\nu} \gamma_{\mu}) (2\delta_{\lambda\mu} - \gamma_{\mu} \gamma_{\lambda})$$

 $= 4\delta_{\mu\nu} \delta_{\nu\mu} - 2\delta_{\mu\nu} \gamma_{\mu} \gamma_{\lambda} - 2\delta_{\lambda\mu} \gamma_{\nu} \gamma_{\mu} + \gamma_{\nu} \gamma_{\mu} \gamma_{\lambda}$
 $= 4\delta_{\nu\lambda} - 2\gamma_{\nu} \gamma_{\lambda} - 2\gamma_{\nu} \gamma_{\lambda} + 4\gamma_{\nu} \gamma_{\lambda} = 4\delta_{\nu\lambda}$.

From it we have $T_r(\gamma_{\mu} \gamma_{\nu} \gamma_{\nu}, \gamma_{\mu}) = 4 T_r(\delta_{\nu}) = 16$.

(iv)
$$\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\rho} \gamma_{\mu} = \gamma_{\mu} (2\delta_{\nu\lambda} - \gamma_{\lambda} \gamma_{\nu}) (2\delta_{\rho\mu} - \gamma_{\mu} \gamma_{\rho})$$

 $= \gamma_{\mu} (4\delta_{\nu\lambda}, \delta_{\rho\mu} - 2\delta_{\nu\lambda} \gamma_{\mu} \gamma_{\rho} - 2\delta_{\rho\mu} \gamma_{\lambda} \gamma_{\nu} + \gamma_{\lambda} \gamma_{\nu} \gamma_{\mu} \gamma_{\rho})$
 $= 4\delta_{\nu\lambda} \gamma_{\rho} - 2\delta_{\nu\lambda} \gamma_{\mu} \gamma_{\mu} \gamma_{\rho} - 2\delta_{\rho\mu} \gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} + \gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} \gamma_{\nu} \gamma_{\rho}$
 $= 4\delta_{\nu\lambda} \gamma_{\rho} - 8\delta_{\nu\lambda} \gamma_{\rho} - 2\gamma_{\rho} \gamma_{\lambda} \gamma_{\nu} + \gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} \gamma_{\mu} \gamma_{\rho}$
 $= -4\delta_{\nu\lambda} \gamma_{\rho} - 2\gamma_{\rho} \gamma_{\lambda} \gamma_{\nu} + \gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} \gamma_{\mu} \gamma_{\rho}$
 $= -4\delta_{\nu\lambda} \gamma_{\rho} - 2\gamma_{\rho} \gamma_{\lambda} \gamma_{\nu} + 4\delta_{\lambda\nu} \gamma_{\rho} \text{ (Using (iii))}$
 $= -2\gamma_{\rho} \gamma_{\lambda} \gamma_{\nu}.$

(v)
$$\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} + \gamma_{\lambda} \gamma_{\nu} \gamma_{\mu} = (2\delta_{\mu\nu} - \gamma_{\nu} \gamma_{\mu}) \gamma_{\lambda} + (2\delta_{\nu\lambda} - \gamma_{\nu}\gamma_{\lambda}) \gamma_{\mu}$$

 $= 2\delta_{\mu\nu} \gamma_{\lambda} + 2\delta_{\nu\lambda} \gamma_{\mu} - \gamma_{\nu} (\gamma_{\mu}\gamma_{\lambda} + \gamma_{\lambda} \gamma_{\mu})$
 $= 2\delta_{\mu\nu} \gamma_{\lambda} + 2\delta_{\nu\lambda} \gamma_{\mu} - 2\delta_{\mu\lambda} \gamma_{\nu}.$

Problem 9. Show that

(i)
$$T_r (\gamma_\mu \gamma_\nu) = 4 \delta_{\mu\nu}$$

(ii)
$$T_r (\gamma_\mu \gamma_\nu \gamma_\lambda) = 0$$

(iii)
$$T_r (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\rho}) = 4\delta_{\mu\nu} \delta_{\lambda\rho} - 4\delta_{\mu\lambda} \delta_{\nu\rho} + 4\delta_{\mu\rho} \delta_{\nu\lambda}$$

(iv)
$$T_r (\gamma_5 \gamma_\mu \gamma_\nu) = 0$$

(v)
$$T_r (\gamma_5 \gamma_\mu \gamma_\nu \gamma_\lambda \gamma_\rho) = 4 \epsilon_{\mu\nu\lambda\rho}$$

Sol.

(i)
$$T_r (\gamma_{\mu} \gamma_{\nu}) = T_r (\gamma_{\nu} \gamma_{\mu}) = \frac{1}{2} T_r (\gamma_{\mu} \gamma_{\nu} + \gamma_{\nu} \gamma_{\mu})$$

 $= \delta_{\mu\nu} T_r I = 4\delta_{\nu\mu}.$

(ii) From
$$\gamma_5 \gamma_\mu + \gamma_\mu \gamma_5 = 0$$
 we have $\gamma_5 \gamma_\mu \gamma_5^{-1} = -\gamma_\mu$

Now taking the trace of both sides and making use of the fact that cyclic permutation does not change the trace, we have

$$-(1)^{3} T_{r} (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda}) = T_{r} (\gamma_{5} \gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{5}^{-1})$$

$$= T_{r} (\gamma_{5}^{-1} \gamma_{5} \gamma_{\mu} \gamma_{\nu} \gamma_{\lambda})$$

$$= T_{r} (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda})$$

$$\Rightarrow T_{r} (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda}) = 0.$$

This result can be generalized to the product of any odd number of gamma matrices other than γ_5 .

(iii)
$$T_r (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\rho}) = 2\delta_{\mu\nu} T_r (\gamma_{\lambda} \gamma_{\rho}) - T_r (\gamma_{\nu} \gamma_{\mu} \gamma_{\lambda} \gamma_{\rho})$$

 $\{ : \gamma_{\mu} \gamma_{\nu} = 2\delta_{\mu\nu} - \gamma_{\nu} \gamma_{\mu} \}$

$$=2\delta_{\mu\nu}T_{\tau}(\gamma_{\lambda}\gamma_{\rho})-2\delta_{\mu\lambda}T_{\tau}(\gamma_{\nu}\gamma_{\rho})+T_{\tau}(\gamma_{\nu}\gamma_{\lambda}\gamma_{\mu}\gamma_{\rho})$$

$$=2\delta_{\mu\nu}T_{\tau}(\gamma_{\lambda}\gamma_{\rho})-2\delta_{\mu\lambda}T_{\tau}(\gamma_{\nu}\gamma_{\rho})+2\delta_{\mu\rho}T_{\tau}(\gamma_{\nu}\gamma_{\lambda})$$

$$-T_{\tau}(\gamma_{\nu}\gamma_{\lambda}\gamma_{\rho}\gamma_{\mu})$$

or
$$2T_r (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\rho}) = 2\delta_{\mu\nu} T_r (\gamma_{\lambda} \gamma_{\rho}) - 2\delta_{\mu\lambda} T_r (\gamma_{\nu} \gamma_{\rho})$$

 $+ 2\delta_{\mu\rho} T_r (\gamma_{\nu} \gamma_{\lambda}) \{ : T_r (ABCD) = T_r (DCBA) \}$
 $= 8\delta_{\mu\nu} \delta_{\lambda\rho} - 8\delta_{\mu\lambda} \delta_{\nu\rho} + 8\delta_{\mu\rho} \delta_{\nu\lambda}$

$$T_r (\gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\rho}) = 4\delta_{\mu\nu} \delta_{\lambda\rho} - 4\delta_{\mu\lambda} \delta_{\nu\rho} + 4\delta_{\mu\rho} \delta_{\nu\lambda}$$

(iv) Let us choose a γ -matrix different from both γ_{ν} and γ_{ν} (It is possible because there are four gamma matrices) i.e. we choose γ_{λ} such that $\lambda \neq \mu$, ν . Then we shall have

$$\gamma_{\mu} \gamma_{\lambda} + \gamma_{\lambda} \gamma_{\mu} = 0$$
 and $\gamma_{\nu} \gamma_{\lambda} + \gamma_{\lambda} \gamma_{\nu} = 0$...(a)

Also we have $\gamma_{\lambda}^2 = I$. We can thus write

$$T_{r} (\gamma_{5} \gamma_{\mu} \gamma_{\rho}) = T_{r} (\gamma_{5} \gamma_{\mu} \gamma_{\nu} \gamma_{\lambda} \gamma_{\lambda})$$

$$= T_{r} (\gamma_{\lambda} \gamma_{5} \gamma_{\mu} \gamma_{\nu} \gamma_{\lambda})$$

$$= -T_{r} (\gamma_{5} \gamma_{\lambda} \gamma_{\mu} \gamma_{\nu} \gamma_{\lambda})$$

$$= -T_{r} (\gamma_{5} \gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} \gamma_{\lambda})$$

$$= -T_{r} (\gamma_{5} \gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} \gamma_{\lambda})$$
[Using (a)]
$$= -T_{r} (\gamma_{5} \gamma_{\mu} \gamma_{\nu})$$

$$\Rightarrow T_r (\gamma_5 \gamma_\mu \gamma_\nu) = 0.$$

(v) We have
$$T_r (\gamma_5 \gamma_\mu \gamma_\nu \gamma_\lambda \gamma_\rho) = \epsilon_{\mu\nu\lambda\rho} T_r (\gamma_5 \gamma_5)$$

= $4\epsilon_{\mu\nu\lambda\rho}$.

Problem 10. The Feynman's dagger or slash notation is defined as follows:

$$A_{\mu} = \gamma_{\mu} A_{\mu} = \gamma A;$$
 (A is read as A slash)

Use the results of the previous problem to show that

(i) $T_r(AB) = 4A \cdot B$

(ii)
$$T_r (A B C D) = 4 [(A.B) (C.D) - (A.C) (B.D) + (A.D) (B.C)]$$

(iii) $T_r (\gamma_5 A B) = 0$.

Sol.

(i)
$$T_r (A B) = A_\mu B_\nu T_r (\gamma_\mu \gamma_\nu) = A_\mu B_\nu .4\delta_{\mu\nu}$$

= $4A_\mu B_\mu = 4A . B$

(ii)
$$T_{r}$$
 (A B C) = $A_{\mu}B_{\nu}C_{\lambda}D_{\rho}$ T_{r} (γ_{μ} γ_{ν} γ_{λ} γ_{ρ})
= $A_{\mu}B_{\nu}C_{\lambda}D_{\rho}$ [$4\delta_{\mu\nu}$ $\delta_{\lambda\rho}-4\delta_{\mu\lambda}$ $\delta_{\nu\rho}+4\delta_{\mu\rho}$ $\delta_{\nu\lambda}$]
= $4A_{\mu}B_{\mu}C_{\nu}D_{\lambda}-4A_{\mu}B_{\nu}C_{\mu}D_{\nu}+4A_{\mu}B_{\nu}C_{\nu}D_{\mu}$
= 4 [(A.B) (C.D)-(A.C) (B.D)
+ (A.D) (B.C)]

(iii)
$$T_r (\gamma_5 A B) = A_\mu B_\nu T_r (\gamma_5 \gamma_\mu \gamma_\nu) = 0$$
.

Problem 11. Show that

(i)
$$T_r (A_1 A_2 A_3 ... A_{2n}) = T_r (A_{2n} A_{2n-1} ... A_1)$$

(ii)
$$T_r (A_1 A_2 ... A_n) = (A_1 ... A_2) T_r (A_3 A_4 ... A_n) - (A_1 ... A_3) T_r (A_2 A_4 ... A_n) + ... + (A_1 ... A_n) T_r (A_2 A_3 ... A_{n-1})$$
Sol.

Sol.

Sol.

(i) We have
$$\gamma_{\mu} \gamma_{\nu} + \gamma_{\nu} \gamma_{\mu} = 2\delta_{\mu\nu}$$

$$\therefore \gamma_{\mu} \gamma_{\nu} + \gamma_{\nu} \gamma_{\mu} = 2\delta_{\mu\nu}$$

$$\therefore \gamma_{\mu} \gamma_{\nu} + \gamma_{\nu} \gamma_{\mu} = 2\delta_{\mu\nu}$$

Since the complex conjugates satisfy the same commutation relation as γ 's, there exist a similarity transformation of the type:

B†
$$\gamma_{\mu}^* B = \gamma_{\mu}$$
 ...(ii)

Again, taking the transpose of (i), we get

$$\gamma_{\nu} \gamma_{\mu} + \gamma_{\mu} \gamma_{\nu} = 2\delta_{\mu\nu}$$

From it we see that the commutation relation for transposes is the same as for γ_{μ} 's. Hence there exist another similarity transformation of the type

$$C^{-1} \gamma_{\mu} C = -\gamma_{\mu}$$
...(iii)
$$C^{-1} \gamma_{\mu} C = -\gamma_{\mu}$$
... is its own trans-

Since the trace is just a number and hence it is its own transpose Therefore,

$$T_{r} (A_{1} A_{2}...A_{2n}) = T_{r} (A_{1} A_{2}...A_{2n})$$

$$= T_{r} (A_{2n} A_{2n-1}...A_{1})$$

$$= (-1)^{2n} T_{r} [C A_{2n} C^{-1}.C A_{2n}^{-1}...C A_{1} C^{-1}]$$

$$= T_{r} [C A_{2n} A_{2n-1}...A_{1} C^{-1}]$$

$$= T_{r} [C^{-1}C A_{2n} A_{2n-1}...A_{1}]$$

$$= T_{r} [A_{2n} A_{2n-1}...A_{1}].$$

$$= T_{r} [A_{2n} A_{2n-1}...A_{1}].$$

(ii) $T_r (A_1 A_2 ... A_n) = 2A_1 A_2 T_r (A_3 ... A_n) - T_r (A_2 A_1 A_3 ... A_n)$ To write it we have used:

$$A_1A_2 = -A_2A_1 + 2A_1A_2$$

Continuing like this we get the required result.

Problem 12. Consider the following set of 16 elements

 $\gamma_1, \gamma_2, \gamma_3, \gamma_4$ $i\gamma_1\gamma_3$, $i\gamma_2\gamma_1$, $i\gamma_3\gamma_2$, $i\gamma_1\gamma_4$, $i\gamma_2\gamma_4$, $i\gamma_3\gamma_4$ $i\gamma_1\gamma_2\gamma_3$, $i\gamma_2\gamma_1\gamma_4$, $i\gamma_3\gamma_2\gamma_4$, $i\gamma_3\gamma_1\gamma_4$

Denoting the elements of the set by Γ_A , A=1, 2,..., 16, verify that they have the following properties:

 $\Gamma^2 A = 1$.

The product of any two elements of the set is proportional (ii) to a third element of the set,

i.e.
$$\Gamma_A \Gamma_B = a \Gamma_C$$

114 (iii) If
$$\Gamma_A \neq I$$
, then Γ_B can always be found such that $\Gamma_B \Gamma_A \Gamma_B = -\Gamma_A$.

(iv) If $\Gamma_A \neq I$, then $T_r(\Gamma_A) = 0$

(1V) All the Γ_A 's are linearly independent.

(V) Γ_A and Γ_A are linearly independent. (vi) If a matrix commutes with all the T's, then it is a constant (vi) If a matrix.

multiple of the unit matrix. Relation (i) to (iii) can be verified by direct calculation sol. Soi.

using the commutation rules of y's. For example, with the

 $\Gamma_6 = i\gamma_1\gamma_3$, $\Gamma_{16} = \gamma_1\gamma_2\gamma_3\gamma_4 = \gamma_5$, we have notations $\Gamma_6\Gamma_{16}\Gamma_6 = -\gamma_1\gamma_3\gamma_5\gamma_1\gamma_3$ $=+\gamma_1\gamma_1\gamma_3\gamma_5\gamma_3$ $=+\gamma_3\gamma_5\gamma_3$ $= -\gamma_3\gamma_3\gamma_5 = -\gamma_5 = -\Gamma_{16}$

Using (iii) we can prove (iv) very easily

For (v) we have to show that

$$\sum_{A=1}^{16} a_A \Gamma_A = 0 \qquad \dots (a)$$

if and only if, all the coefficients a_A (A=1, ... 16) are equal to

By taking the trace of (a), and using the property (iv) we find zero. that $a_1 = 0$.

Similarly, multiplying (a) by Γ_A and using the relations

$$\Gamma_A^2 = 1$$
, $\Gamma_A \Gamma_B = a \Gamma_C \& \Gamma_r (\Gamma_A) = 0$;

we find that $a_A = 0$ for all values of A.

For the last part, let X be a 4×4 matrix which commutes with all the gamma matrices. From the linear independence of the Γ_A 's it follows that X can be written in the form:

$$X = \sum_{A=1}^{16} x_A \Gamma_A \qquad \dots (b)$$

Multiplying boto sides of it by I'a and taking the trace we find

$$x_A = \frac{1}{4} T_r (X\Gamma_A) \qquad \dots (c)$$

Let us now write (b) in the form $X = x_B \Gamma_B + \sum_{C \neq B} x_C \Gamma_C ; \quad \Gamma_B \neq 1 \qquad ...(d)$

Since $\Gamma_B \neq I$, according to part (iii), there exists a matrix Γ_A such that $\Gamma_A \Gamma_B \Gamma_A = -\Gamma_B$. Also, since X commutes with all the Γ 's, we have $\Gamma_A \times \Gamma_A = X$. Now multiplying (d) from left as well as from right by Γ_A and making use of these properties, we get:

$$X = -x_B \Gamma_B + \sum_{C \neq B} x_C \Gamma_A \Gamma_C \Gamma_A$$

$$= -x_B \Gamma_B + \sum_{C \neq B} (\pm 1) x_C \Gamma_C, \qquad \dots (e)$$

in this we have +1 if Γ_C and Γ_A commute, and -1 if they anticommute. If we multiply (d) and (e) by Γ_B , and take the trace, it follows that $x_B = -x_B = 0$.

Since Γ_B could equally well have been any one of the Γ -matrices (excluding I), it follows that the only non-vanishing coefficients in the expression (b) is that of I, a fact which completes the proof of the statement (vi).

Problem 13. Show that γ_5 is a constants of motion for a mass-less Dirac particle

Sol. The Hamiltonian for a zero mass Dirac particle is given by

 $H = -\gamma_5 \sigma' \circ \mathbf{p}$ $\Rightarrow \sigma' = \begin{pmatrix} \sigma & 0 \\ \sigma & \rightarrow \\ 0 & \sigma \end{pmatrix} = -\gamma_5 \alpha$ $\therefore H = -\gamma_5 \cdot -\gamma_5 \alpha \circ \mathbf{p}$ $\Rightarrow \alpha \cdot \mathbf{p}$

Since y₅ commutes with α , therefore,

where

$$[\gamma_5, H] = 0$$

Thus γ_5 is a constant of motion for a zero mass particle.

Problem 14. Calculate the following trace:

$$T_r \left[\gamma_{\mu} \Lambda^{(+)}(p_1) \; \gamma_{\mu} \Lambda^{(+)}(p_1') \right]$$

Sol.
$$T_r \left[\gamma_{\mu} \Lambda^{(+)} (p_1) \gamma_{\mu} \Lambda^{(+)} (p_1') \right]$$

= $T_r \left[\gamma_{\mu} \frac{m - i p_1}{2m} \gamma_{\mu} \frac{m - i p_1'}{2m} \right]$

$$= \frac{1}{4m^2} \left[m^2 T_r (\gamma_{\mu} \gamma_{\mu}) - T_r (\gamma_{\mu} p_1 \gamma_{\mu} p_1') \right] ...(i)$$

Here we have used the fact that the trace of the product of an odd number of gamma matrices vanishes.

Now,
$$T_r (\gamma_{\mu}\gamma_{\mu})=4$$

and $T_r (\gamma_{\mu}p_1\gamma_{\mu}p_1')=(p_1)_{\nu} (p_1')_{\lambda} T_r (\gamma_{\mu}\gamma_{\nu}\gamma_{\mu}\gamma_{\lambda})$
 $=(p_1)_{\nu} (p_1')_{\lambda} T_r . (-2\gamma_{\nu}\gamma_{\lambda})$
 $=-8\delta_{\nu\lambda} (p_1)_{\nu} (p_1')_{\lambda}$
 $=-8p_1.p_1'$

$$T_r \left[\gamma_{\mu} \Lambda^{(+)} \left(p_1 \right) \gamma_{\mu} \Lambda^{(+)} \left(p_1' \right) \right] = \frac{1}{m^2} \left[m^2 + 2p_1 . p_1' \right]$$

Problem 15. How does the Dirac invariants,

 $S=\bar{\psi}\psi$, $V_{\mu}=\bar{\psi}\gamma_{\mu}\psi$, $T_{\mu\nu}=\bar{\psi}\sigma_{\mu\nu}\psi$, $A_{\mu}=i\bar{\psi}\gamma_{5}\gamma_{\mu}\psi$ and $P=\bar{\psi}\gamma_{5}\psi$ changes under the operations time reversal and the charge conjugation.

Sol. The time reversal is given by operator B with the properties:

$$\psi'(x') = B\psi^*(x) ;$$

$$E\gamma_{\mu}^* B^{-1} = \gamma_{\mu} ;$$

$$\psi'(x') = \psi^*(x) B^{-1}$$
...(i)

and

The charge conjugation is given by the operation of the matrix C with the properties:

$$\frac{\psi^{c} = C\widetilde{\psi}}{C\widetilde{\gamma}_{\mu}C^{-1} = -\gamma_{\mu}} \left. \begin{array}{c} \\ \\ \\ \overline{\psi^{c}} = -\widetilde{\psi}C^{-1} \end{array} \right\} \dots (ii)$$

and

Hence under time reversal,

$$S' = \overline{\psi}' \psi' = \overline{\psi}^* B^{-1} B \psi^* = \overline{\psi}^* \psi^* = (\overline{\psi}\psi)^* = S^*$$

$$V_{\mu}' = \bar{\psi}' \gamma_{\mu} \psi' = \bar{\psi}^* B^{-1} \gamma_{\mu} B \psi^* = \bar{\psi}^* B^{-1} (B \gamma_{\mu}^* B^{-1}) B \psi^*$$

$$= \bar{\psi}^* \gamma_{\mu}^* \psi^* = (\bar{\psi} \gamma_{\mu} \psi)^* = V_{\mu}^*$$

$$T'_{\mu\nu} = \frac{\overline{\psi'}}{2i} (\gamma_{\mu}\gamma_{\nu} - \gamma_{\nu}\gamma_{\mu}) \psi'$$

$$= \frac{\overline{\Psi^*B^{-1}}}{2i} \left(\gamma_{\mu} \gamma_{\nu} - \gamma_{\nu} \gamma_{\mu} \right) B \Psi^*$$

$$= \frac{\overline{\psi}^*}{2i} \left\{ B^{-1} \gamma_{\mu} B B^{-1} \gamma_{\nu} B - B^{-1} \gamma_{\nu} B B^{-1} \gamma_{\mu} B \right\} \psi^*$$

Similarly, $P' = P^*$.

To find the transformation under the charge conjugation we first antisymmetrise the covariant and then find its transformed form; therefore,

and

$$S = \frac{1}{2} \left[\overline{\psi}_{\alpha} \psi_{\beta} - \psi_{\beta} \overline{\psi}_{\alpha} \right]$$

$$S^{c} = \frac{1}{2} \left[\overline{\psi}_{\alpha}^{c} \psi_{\beta}^{c} - \psi_{\beta}^{c} \overline{\psi}_{\alpha}^{c} \right]$$

$$= \frac{1}{2} \left[\overline{\psi}_{\alpha}^{c} \psi_{\beta}^{c} - (\overline{\psi}_{\beta}^{c} \overline{\psi}_{\alpha}^{c}) \right]$$

$$= \frac{1}{2} \left[-\overline{\psi}_{\alpha} C^{-1} \cdot C \overline{\psi}_{\beta} + (\overline{\psi}_{\beta} C^{-1} \cdot C \overline{\psi}) \right]$$

$$= \frac{1}{2} \left[-\overline{\psi}_{\beta} \psi_{\alpha} + \overline{\psi}_{\beta} \psi_{\alpha} \right]$$

$$= \frac{1}{2} \left[\overline{\psi} \psi - \overline{\psi} \psi \right] = S$$

$$V_{\mu} = \overline{\psi}_{\mu}\psi = \frac{1}{2} \left[\overline{\psi}_{\alpha} (\gamma_{\mu})_{\alpha\beta}\psi_{\beta} - \psi_{\beta} (\gamma_{\mu})_{\beta\alpha}\overline{\psi}_{\alpha} \right]$$

$$= \frac{1}{2} \left[\overline{\psi}_{\alpha}(\gamma_{\mu})_{\alpha\beta}\psi_{\beta} - \overline{\psi}_{\alpha}(\gamma_{\mu})_{\alpha\beta}\psi_{\beta} \right]$$

$$= \frac{1}{2} \left[\overline{\psi}(\gamma_{\mu}\psi) - (\overline{\psi}_{\gamma_{\mu}}\psi) \right]$$

.. $V_{\mu}^{c} = V_{\mu}$, as in the case of j_{μ} .

$$P = \bar{\psi}\gamma_5\psi = \bar{\psi}_{\alpha}(\gamma_5)_{\alpha\beta}\psi_{\beta}$$

$$= \frac{1}{2} \left[\bar{\psi}\gamma_{\alpha}\psi - (\bar{\psi}\gamma_5\psi) \right]$$

$$P^{c} = \frac{1}{2} \left[\overline{\psi}_{c} \gamma_{5} \psi^{c} - (\overline{\psi}^{c} \gamma_{5} \psi^{c}) \right]$$

$$= \frac{1}{2} \left[-\widetilde{\psi} C^{-1} \gamma_{5} C \overline{\psi} + (\widetilde{\psi} C^{-1} \gamma_{5} C \overline{\psi}) \right]$$

$$= \frac{1}{2} \left[-\widetilde{\psi} \gamma_{5} \overline{\psi} + (\overline{\psi} \gamma_{5} \overline{\psi}) \right]$$

$$= \frac{1}{2} \left[\overline{\psi} \gamma_{5} \psi - (\overline{\psi} \gamma_{5} \psi) \right] = P$$

Similarly, we find that $A_{\mu} \circ = -A_{\mu}$

Lastly we have $T_{\mu\nu} = \overline{\psi} \sigma_{\mu\nu} \psi$

$$=\frac{1}{2i}\left[\bar{\Psi}\,\gamma_{\mu}\gamma_{\nu}\psi-\bar{\Psi}\,\gamma_{\nu}\gamma_{\mu}\psi\right]$$

$$= \frac{1}{2i} \left\{ \frac{1}{2} \left[\overline{\psi}_{\alpha} \left(\gamma_{\mu} \gamma_{\nu} \right)_{\alpha \beta} \psi_{\beta} - \psi_{\beta} \left(\gamma_{\mu} \gamma_{\nu} \right)_{\beta \alpha} \overline{\psi}_{\alpha} \right] \right.$$

$$\left. - \frac{1}{2} \left[\overline{\psi}_{\alpha} \left(\gamma_{\nu} \gamma_{\mu} \right)_{\alpha \beta} \psi_{\beta} - \psi_{\beta} \left(\gamma_{\nu} \gamma_{\mu} \right)_{\beta \alpha} \overline{\psi}_{\alpha} \right] \right\}$$

$$= \frac{1}{4i} \left\{ \left[\overline{\psi} \gamma_{\mu} \gamma_{\nu} \psi - \left(\overline{\psi} \gamma_{\mu} \gamma_{\nu} \psi \right)^{2} \right]$$

$$-\left[\bar{\psi}\,\gamma_{\nu}\gamma_{\mu}\psi - (\bar{\psi}\,\gamma_{\nu}\gamma_{\mu}\psi)\right]\}$$

$$T^{c}_{\mu\nu} = \frac{1}{4i} \left\{ \left[\bar{\psi}^{c}\,\gamma_{\mu}\gamma_{\nu}\,\psi^{c} - (\bar{\psi}^{c}\,\gamma_{\mu}\gamma_{\nu}\psi^{c})\right]\right\}$$

$$-[\overline{\psi}^{c} \gamma_{\nu} \gamma_{\mu} \psi^{c} - (\overline{\psi}^{c} \gamma_{\nu} \gamma_{\mu} \psi_{c})]$$

Let us consider the term

$$\overline{\Psi}^{c} \gamma_{\mu} \gamma_{\nu} \Psi_{c} = -\overline{\Psi} C^{-1} \gamma_{\mu} \gamma_{\nu} C \overline{\Psi}$$

$$= -\overline{\Psi} C^{-1} \gamma_{\mu} C. C^{-1} \gamma_{\nu} C \overline{\Psi}$$

$$= -\overline{\Psi} \gamma_{\mu} \widetilde{\gamma}_{\nu} \widetilde{\Psi} = -(\widetilde{\Psi} \gamma_{\nu} \gamma_{\mu} \Psi)$$

Similarly, evaluating the other terms we find that

$$T_{\mu\nu}^{c} = -T_{\mu\nu}$$

Problem 16. Find out ψ_{PCT} , i.e., ψ after applying successively the transformations T, C and P. Hence show that the Dirac equation

$$[-i\alpha.(\nabla+ieA)+\beta m-eA_0]\psi=-E\psi \qquad ...(i) \ \neg$$

changes into

$$[+i\alpha.(\nabla + ieA) + \beta m - eA_0] \psi_{PCT} = E\psi_{PCT} \qquad ...(ii)$$

under these transformations. Interprete the results.

Sol. We have

$$\psi_P = e^{i\xi} \gamma_4 \psi$$
; $\psi_T = (\gamma_4 \gamma_5 \gamma_2) \psi^*$ and $\psi_C = (\gamma_4 \gamma_2) \psi^*$

:. $\psi_{PC}=e^{i\xi}\left(\gamma_4\gamma_2\right)\gamma_4\tilde{\psi}=-e^{i\xi}\gamma_4\gamma_4\gamma_2\tilde{\psi}=-e^{-i\xi}\gamma_2\tilde{\psi}$ and hence,

$$\begin{split} \psi_{PCT} &= (\gamma_4 \gamma_5 \gamma_2) \cdot (-e^{i\xi} \gamma_2 \tilde{\psi})^* \\ &= -\gamma_4 \gamma_5 \gamma_2 \gamma_2 \cdot e^{i\xi} (\tilde{\psi})^* \\ &= -\gamma_4 \gamma_5 \gamma_4 e^{i\xi} \psi \, \{ \because \; \tilde{\psi} = \psi \; \gamma_4 = \tilde{\psi}^* \gamma_4 \Rightarrow (\tilde{\psi})^* = \gamma_4 \psi \} \\ &= e^{i\xi} \gamma_5 \psi \end{split}$$

Taking the arbitrary phase factor eit as unity we have:

$$\psi_{PCT} = \gamma_5 \psi \qquad ...(iii)$$

Now we find the transformation of (i) under PCT. Under (PT)-transformation, i.e., space-time co-ordinate inversions, x_{μ} and A_{μ} transforms as:

$$\left.\begin{array}{l}
\chi_{\mu} \to \chi_{\mu}' = -\chi_{\mu} \\
A_{\mu} \to A_{\mu}' = A_{\mu}
\end{array}\right\} \dots (iv)$$

while there is no change in x_{μ} and A_{μ} due to C-transformation.

Also from (iii) we have $\psi = \gamma_5 \psi_{PCT}$...(v)

Using (iv) and (v) into (i) we get it after PCT-transformation as:

$$[-i\alpha.(-\nabla'-ie\ A')+\beta m+eA'o]\ \gamma_5\ \psi_{PCT}(x')=-E\gamma_5\ \psi_{PCT}(x')$$

or
$$\gamma_5 \left[-i \alpha \cdot (-\nabla' - ieA') + \beta m + eA_0' \right] \gamma_5 \psi_{PCT}(x') = -E\gamma_5^2 \psi_{PCT}(x')$$

or
$$[i \alpha.(-\nabla'-ieA')-\beta m+eA_0'] \psi_{PCT}(x')=-E \psi_{PCT}(x')$$

or
$$[+i\alpha.(\nabla'+ieA')+\beta m-eA_0']\psi_{PCT}(x')=E\psi_{PCT}(x')$$
.

or deleting the primes,

$$[i \stackrel{\rightarrow}{\alpha} (\nabla' + ieA) + \beta m - eA_0] \psi_{PCT} (x) = E \psi_{PCT} (\alpha) \qquad ...(vi)$$

Comparing (vi) with (i) we find that a negative energy electron moving backward in space-time is a positive energy particle moving positively in space time. This interpretation of the positron as negative energy electron running backward in time, forms the basis of Feynman's theory of positron to be discussed in the next chapter.

In scattering problems we look for the solutions of the wave-equation which develop in time from some initial state in the remote past; i.e., given the wavefunction for a particle in the remote past, we want to know it in the far future after its interaction with a potential.

According to Huygen's principle, if the wavefunction ψ (x_1 , t_1) is known at a particular time t_1 , it may be found at any later time t_2 by considering at time t_1 each point of space, x_1 , as a source of secondary wavelets, which propagate outward from x_1 . The strength of the wave amplitude at any point x_2 at a later time t_2 will be proportional to the original wave amplitude ψ (x_1 , t_1). If we denote the constant of proportionality per unit volume around the point x_1 by K (x_2 , t_2 ; x_1 , t_1), the total wave arriving at (x_2 , t_2) will be

$$\psi(\mathbf{x}_{2}, t_{2}) = \int d^{3}x_{1} K(\mathbf{x}_{2}, t_{2}; \mathbf{x}_{1}, t_{1}) \psi(\mathbf{x}_{1}, t_{1}); t_{2} \geq t_{1}, \dots (1)$$

where the integration is taken over the entire space from which the secondary waves are emitted. $K(\mathbf{x}_2, t_2; \mathbf{x}_1, t_1)$ is called the "Green's function" or Propagator" for eqn. (1). Knowledge of K enables us to construct the physical state which develops in time from any given initial state, and thus, it is equivalent to a complete solution of the equation of motion.

The Propagator method due to Feynman simplifies very much the calcutions involving positrons and electrons interacting with an external field. Later, after developing the subject of field quantization in chapter 13, we shall clearly see the equivalence of Feynman's formulation to the more standard field theoretic approach. We present this approach in some detail here, because it will provide an intuitive understanding of the essentials of the field-theoretic results to be derived rigorously later on.

11.1. PROPAGATOR FOR A NONRELATIVISTIC SCHRO-DINGER FREE PARTICLE:

We have the Schroedinger equation in the natural units as:

$$\frac{i \partial \psi (\mathbf{x}, t)}{\partial t} = H\psi (\mathbf{x}, t) \qquad \dots (2)$$

We now want to transform it into the integral form (1). For it we expand $\psi(x, t)$ in terms of the complete set of orthonormal eigenfunctions $u_n(x)$ of the time independent Hermitian operator H with eigenvalues E_n ,

$$E_n u_n(\mathbf{x}) = H u_n(\mathbf{x}) \qquad \dots (3)$$

Functions un satisfy the relations (See prob. 2, Chapter-2),

$$\int u_n^* (x) u_m (x) d^3x = \delta_{nm}; \sum_n u_n (x) u_n^* (x') = \delta^3 (x - x').$$

(orthonormality relation) (completeness relation)

We can now expand $\psi(\mathbf{x}_2, t)$ as (See eqn. (90), chapter-1):

$$\psi(\mathbf{x}_2, t_2) = \sum_{n} a_n u_n(\mathbf{x}_2) \exp(-iE_n t_2)$$
 ...(4)

where,

$$a_n = \int u_n^* (x_1) \psi (x_1, t_1) \exp. (+iE_n t_1) d^3x_1$$

Substituting the value of a_n into (4), we get

$$\psi(\mathbf{X}_{2}, t_{2}) = \sum_{n} \left\{ \int u_{n}^{*}(\mathbf{X}_{1}) \psi(\mathbf{X}_{1}, t_{1}) \exp(iE_{n}t_{1}) d^{3}x_{1} \right\} \times u_{n}(\mathbf{X}_{2}) \exp(-iE_{n}t_{2})$$

$$= \int d^3x_1 \left\{ \sum_{n} u_n^* (\mathbf{x}_1) \ u_n (\mathbf{x}_2) \ \exp \left[-iE_n (t_2 - t_1)\right] \right\} \psi (\mathbf{x}_1, t_1)$$

In order to compare this equation with eqn. (1), we have to incorporate the condition that $t_2 \ge t_1$. We introduce a step function $\theta(t)$ defined by

$$\theta(t) = \begin{cases} 1 & \text{if } t \ge 0 \\ 0 & \text{if } t < 0 \end{cases} \dots (6)$$

and write

$$\psi(\mathbf{x}_{2}, t_{2}) = \int d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \{ \sum_{n} u_{n} * (\mathbf{x}_{1}) u_{n} (\mathbf{x}_{2}) \exp[-iE_{n} (t_{2} - t_{1})] \theta(t_{2} - t_{1}) \} \times d^{3}x_{1} \}$$

Condition $t_2 \ge t_1$ incorporated into (5) has to be for the conservation of casuality. The contribution to the wave ψ (\mathbf{x}_2 , t_2) must come only from the waves ψ (\mathbf{x}_1 , t_1) which were produced earlier in time and not from the waves propagating in future time. Comparing (7) with (1) we find the propagator

$$K(\mathbf{x}_2, t_2; \mathbf{x}_1, t_1) = \sum_{n} u_n^* (\mathbf{x}_1) u_n (\mathbf{x}_2) \exp[-iE_n (t_2 - t_1)] \theta (t_2 - t_1)$$

It is now a simple matter to derive the differential equation 522 satisfied by K: $\left(i\frac{\partial}{\partial t_2}-H_2\right)K\left(\mathbf{x}_2,\,t_2;\,\mathbf{x}_1,\,t_1\right)$ $= i \sum_{n} u_n^* (\mathbf{x}_1) u_n (\mathbf{x}_2) \frac{\partial}{\partial t_2} \{ \exp \left[-iE_n \left(t_2 - t_1 \right) \right] \theta \left(t_2 - t_1 \right) \}$ $-\Sigma u_n^* (\mathbf{x}_1) \{ H_2 u_n (\mathbf{x}_2) \} \exp [-iE_n (t_2-t_1)] \theta (t_2-t_1)$ $= \sum_{n} u_n^* (\mathbf{x}_1) u_n (\mathbf{x}_2) \{ E_n \exp_{-i} [-iE_n (t_2 - t_1)] \theta (t_2 - t_1) \}$ $+i\delta (t_2-t_1) \exp \left[-iE_n (t_2-t_1)\right]$ $-\sum u_n^* (x_1) E_n u_n (x_2) \exp \left\{-iE_n (t_2-t_1)\right\} \theta (t_2-t_1)$ $\left\{ : \frac{d\theta(x)}{dx} = \delta(x) \right\}$ $= \sum u_n^* (\mathbf{x}_1) u_n (\mathbf{x}_2) . i \delta (t_2 - t_1) \exp \left[-iE_n (t_2 - t_1)\right]$

 $=i\delta (t_2-t_1) \sum_n u_n^* (X_1) u_n (X_2)$

{Using completeness of un) $=i\delta (t_2-t_1) \delta^3 (x_2-x_1)$ $=i\delta^4\left(x_2-x_1\right)$

where δ^4 (x_2-x_1) is the four-dimensional Dirac delta function.

Exactly similar to (9) we get

$$\left(i\frac{\partial}{\partial t_1} - H_1\right) K\left(\mathbf{x}_2, t_2; \mathbf{x}_1, t_1\right) = -i\delta^4 \left(\mathbf{x}_2 - \mathbf{x}_1\right) \qquad \dots (10)$$

We now solve explicitly the equation for the free particle The Hamiltonian for a non-relativistic schroedinger's free particle is written as

$$H_2 = \frac{p_2^2}{2m} = -\frac{1}{2m} \cdot \nabla_2^2$$
 ...(11)

Thus the propagator $K(\mathbf{x}_2, t_2; \mathbf{x}_1 t_1)$ (Here after to be denoted by $K(x_2-x_1)$ } satisfies the equation:

$$\left(i\frac{\partial}{\partial t_2} + \frac{1}{2m}\nabla_2^2\right)K(x_2 - x_1) = i\delta^4(x_2 - x_1) \qquad \dots (12)$$

Taking analogy from the 3-dimensional delta function we can represent δ^4 (x_2-x_1) by the following integral

$$\delta^{4} (x_{2} - x_{1}) = \frac{1}{(2\pi)^{4}} \int_{-\infty}^{+\infty} d^{4}p \exp \left[ip \cdot (x_{2} - x_{1})\right] \dots (13)$$
which we

 $\delta^4 (x_2 - x_1) = \frac{1}{(2\pi)^4} \int_{-\infty}^{+\infty} d^4 p \exp \left[ip \cdot (x_2 - x_1)\right] \dots (13)$ Introducing the Fourier transform of $K(x_2 - x_1)$, which we ste by $K(x_1)$ denote by K(p), as fallows

$$K(x_2-x_1) = \frac{1}{(2\pi)^4} \int d^4p \exp \left[ip. (x_2-x_1)\right] K(p)$$

$$= \frac{1}{(2\pi)^4} \int d^4p \exp \left[ip. (x_2-x_1)-i\omega (t_2-t_1)\right] K(p),$$
...(14)

and using (13) and (14) into (12), we get the equation for K(p) as:

$$\left(\omega - \frac{p^2}{2m}\right) K(p) = i$$

$$\therefore K(p) = \frac{i}{\omega - p^2/2m} \qquad \dots (15)$$

Hence, from eqn. (14) we write

-1

$$K(x_2-x_1) = \frac{i}{(2\pi)^4} \int d^4p \exp \left[i\mathbf{p} \cdot (\mathbf{x}_2-\mathbf{x}_1) - i\omega \left(t_2-t_1\right)\right] \frac{1}{\omega - p^2/2m} \dots (16)$$

The integral on the right has got a singularity at $\omega = p^2/2m$ on the real axis. According to "Jordan's lemma*, we choose the contour for the evaluation of (16) as show in the following diagram. [Fig. (1)].

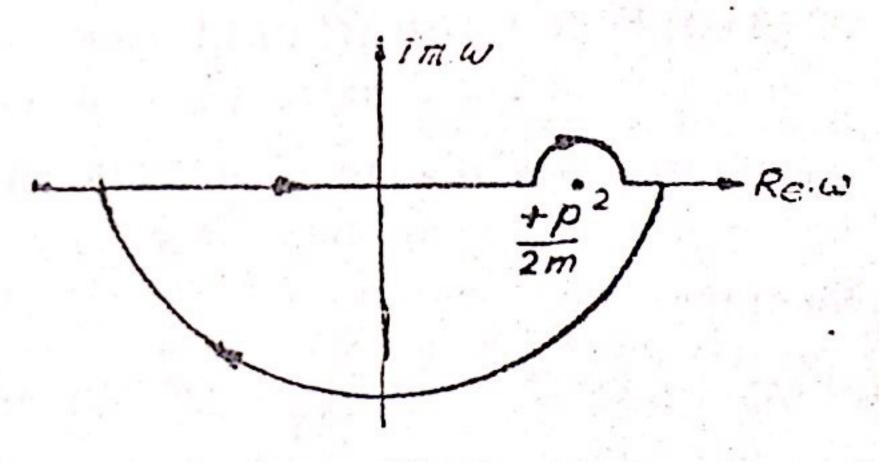


Fig. 1.

Hence the ω integral in (16) can be evaluated by using the Residue theorem as

$$K (x_2-x_1) = \frac{i}{(2\pi)^4} \int d^3p \ d\omega \ \exp. \left[i\mathbf{p}.(\mathbf{x}_2-\mathbf{x}_1) - i\omega \ (t_2-t_1) \right] \frac{1}{\omega - p^2/2m}$$

$$= \frac{i}{(2\pi)^4} \int d^3p \ \exp. \left[i\mathbf{p}.(\mathbf{x}_2-\mathbf{x}_1) \right]$$

$$\times (-2\pi i) \ \text{Res.}$$

$$\omega = p^2/2m \left[\exp. \left\{ -i\omega \ (t_2-t_1) \right\} \frac{1}{\omega - p^2/2m} \right]$$

^{*}According to Jordan's lemma, the function exp. (imz)f(z) can be integrated over a semicircular contour which must be in the upper half or the lower half complex z-plance according as m is positive or negative. In (16), for the ω -integral we have $m=-(t_2-t_1)$ which is negative for $t_2 > t_1$, hence we have closed the contour in the lower half of the complex ω -plane.

$$= \frac{1}{(2\pi)^3} \int d^3p \exp \left[i\mathbf{p} \cdot (\mathbf{x}_2 - \mathbf{x}_1)\right].$$

$$\times \exp \left[(-ip^2/2m) (t_2 - t_1)\right]; t_2 \ge t_1,$$

or
$$K(x_2-x_1) = \frac{1}{(2\pi)^3} \int d^3p \exp[i\mathbf{p}.(\mathbf{x_2}-\mathbf{x_1})]$$

 $\times \exp[(-ip^2/2m)(t_2-t_1)] \delta(t_2-t_1) \dots (17)$

This is the explicit form of the Propagator for a non-

relativistic free particle. Since the propagator $K(x_2-x_1)$ represents a free particle travelling from the point (x_1,t_1) to (x_2, t_2) in the space-time coordinates it can be represented by a straight line (fig. 2) in the space time diagram (Feynman's diagrams).

We could also get $K(x_2-x_1)$ by solving equation (10) and it is left as an exercise for the readers to show that we get exactly the same propagator from (10) by taking

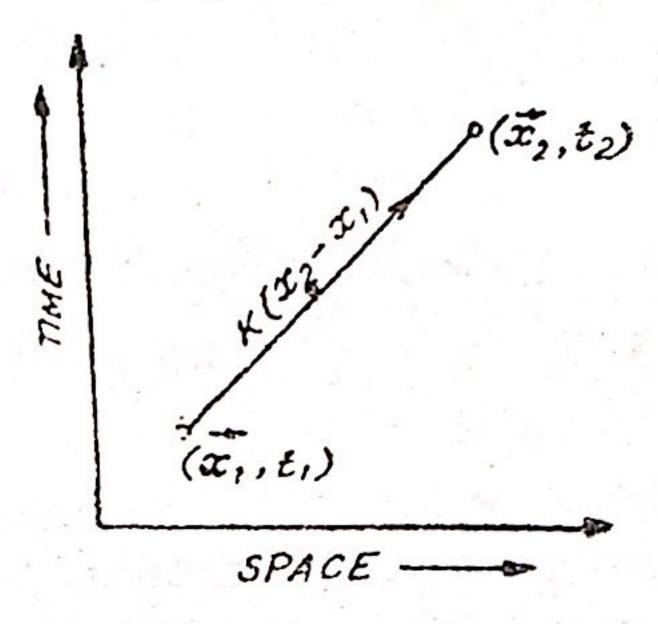


Fig. 2

same propagator from (10) by taking $H_1 = (-1/2m) \nabla_{1}^{2}$.

11.2. PROPAGATOR FOR A DIRAC FREE PARTICLE:

It has been shown in the last chapter that the complete set of the energy eigenfunctions of the Dirac Hamiltonian $H = \alpha$. p $+\beta m$ is given by:

For positive energy:

$$\frac{1}{\sqrt{(V)}}u^{r} \text{ (p) exp. } \{ip.x-iEpt\} \equiv \frac{1}{\sqrt{(V)}}u^{r} \text{ (p) exp. } \{ip.x\} \text{ (r=1, 2)}$$

For negative energy:

$$\frac{1}{\sqrt{(V)}} v^{r}(\mathbf{p}) \exp. \{i\mathbf{p}.\mathbf{x} + iE_{p}t\} \equiv \frac{1}{\sqrt{(V)}} v^{r}(p) \exp. \{i\mathbf{p}.\mathbf{x}\} (r=1,2)$$

where the spinors $u^r(p)$ and $v^r(p)$ satisfy the eqns:

$$(\alpha.p + \beta m) u^r (p) = E_p u^r (p)$$

$$(\alpha.p + \beta m) v^r (p) = -E_p v^r (p).$$

Performing the steps analogous to steps (4) through (8) in the last section, we find that the propagator for the free Dirac particle can be written as:

$$K(x_{2}-x_{1}) = \sum_{i} \frac{1}{V} \left\{ u^{r}(p) u^{r} + (p) - v^{r}(p) v^{r} + (p) \right\} \times$$

$$= r, p \qquad \text{exp. } \{ip. (x_{2}-x_{1})\} \theta (t_{2}-t_{1})$$

To derive the equations satisfied by $K(x_2-x_1)$ we have:

$$\begin{pmatrix} i \frac{\partial}{\partial t_2} - H_2 \end{pmatrix} K(x_2 - x_1) = \begin{pmatrix} i \frac{\partial}{\partial t_2} - \alpha \cdot \mathbf{p}_2 - \beta m \end{pmatrix} K(x_2 - x_1) \\
= \frac{i}{V} \sum_{r, p} \{ u^r(p) u^r \dagger(p) v^r(p) v^r \dagger(p) \}$$
(in (v. x.)) $\delta(t - x_1) = \delta(t - x_2)$

 $\times \exp \{ip.(x_2-x_1)\} \delta(t_2-t_1)$

Using the completeness relation,

$$\sum_{r} [u^{r}(p) \bar{u}^{r}(p) - v^{r}(p) \bar{v}^{r}(p)] = 1,$$

we can write the above eqn. as:

$$\left(\begin{array}{c} i\frac{\partial}{\partial t_{2}} + i \stackrel{\longrightarrow}{\alpha} \cdot \nabla_{2} - \beta m \end{array} \right) K \left(x_{2} - x_{1} \right)$$

$$= \frac{i}{V} \sum_{p} \gamma_{4} \exp \left\{ i \mathbf{p} \cdot (\mathbf{x}_{2} - \mathbf{x}_{1}) \right\} \delta \left(t_{2} - t_{1} \right)$$

$$= i \gamma_{4} \delta^{3} \left(\mathbf{x}_{2} - \mathbf{x}_{1} \right) \delta \left(t_{2} - t_{1} \right)$$

$$\left\{ \begin{array}{c} \vdots & \frac{1}{V} \sum_{p} \Leftrightarrow \frac{1}{(2\pi)^{3}} \int d^{3} p \end{array} \right\}$$

or
$$\left(i\frac{\partial}{\partial t_2}\overrightarrow{i}\alpha.\nabla_2-\gamma_4m\right)$$
 $K(x_2-x_1)=i\gamma_4\delta^4(x_2-x_1)$ $\{::\beta\equiv\gamma_4\}$

Multiplying its both sides by 24 from left we get

$$\left(i \gamma_{4} \frac{\partial}{\partial t_{2}} + i \gamma_{4} \stackrel{\rightarrow}{\alpha} \cdot \nabla_{2} - m\right) K \left(x_{2} - x_{1}\right) = i\delta^{4} \left(x_{2} - x_{1}\right)$$
or
$$\left(-\gamma^{4} \frac{\partial}{\partial (x_{4})_{2}} \stackrel{\rightarrow}{-\gamma} \cdot \nabla_{2} - m\right) K \left(x_{2} - x_{1}\right) = i\delta^{4} \left(x_{2} - x_{1}\right)$$

$$\left(:: \gamma i = -i\gamma_{4} \alpha_{i} \right)$$

or
$$\left(\gamma_{\mu} \frac{\partial}{\partial (x_{\mu})_{2}} + m\right) K (x_{2} - x_{1}) = -i\delta^{4} (x_{2} - x_{1})$$

or $(\partial_{2} + m) K (x_{2} - x_{1}) = -i\delta^{4} (x_{2} - x_{1})$...(18a)

where

$$\mathfrak{F}_2 = \gamma_\mu \frac{\partial}{\partial (x_\mu)_2}$$

Similarly, it can be shown that

$$(\mathcal{J}_1 - m) K (x_2 - x_1) = i\delta^4 (x_2 - x_1)$$
 ...(18b)

These are the differential equations for $K(x_2-x_1)$. The find an explicit solution of (18a) (say), we write the four-dimensional delta function as:

$$\delta^4 (x_2 - x_1) = \frac{1}{(4\pi)^4} \int d^4 p \exp \{ip.(x_2 - x_1)\} \qquad ...(19)$$

Also, introducing the Fourier transform of $K(x_2-x_1)$, which we denote by K(p), we have 526

$$\frac{\int_{e}^{A150} de^{\text{note}} \text{ by } K(p), \frac{1}{1}}{\int_{e}^{4} (2\pi)^{4}} \int_{e}^{4} \exp \left\{ ip. (x_{2} - x_{1}) \right\} K(p) d^{4}p \qquad ...(20)$$

$$K(x_{2} - x_{1}) = \frac{1}{(2\pi)^{4}} \int_{e}^{4} \exp \left\{ ip. (x_{2} - x_{1}) \right\} K(p) d^{4}p \qquad ...(20)$$

Using (19) and (20) into (18a) we obtain:

$$(ip+m) K(p) = -i \Rightarrow K(p) = \frac{-i}{ip+m} = \frac{-i(m-ip)}{p^2+m^2}$$

$$K(x_2-x_1) = \frac{-i}{(2\pi)^4} \int \frac{m-ip}{p^2+m^2} \exp_{-i}\{ip.(x_2-x_1)\} d^4p \qquad ...(21)$$
...

If is convenient to define the integral $I(x_2-x_1)$:

$$I(x_2-x_1) = \frac{-i}{(2\pi)^4} \int \frac{\exp.\{ip.(x_2-x_1)\}}{p^2+m^2} d^4p \qquad \dots (22)$$

$$K(x_2-x_1) = (m-ip) I(x_2-x_1)$$
...(23)
...(23) into (18a) we find that $I(x_2-x_1)$ satisfies.

Inserting (23) into (18a) we find that $I(x_2-x_1)$ satisfies:

$$\lim_{(\square_2^2 - m^2)} I(x_2 - x_1) = i\delta^4 (x_2 - x_1) \qquad \dots (24)$$

where
$$\Box_2^2 = \partial_2^2 = \nabla_2^2 - \frac{\partial^2}{\partial t_2}$$
 ...(25)

Eqn. (24) is an inhomogeneous Klein-Gordon equation and hence we can interprete $I(x_2-x_1)$ as the propagator for the zero spin K.G. free particle.

In the integral (22), there are two simple poles on the real

axis, given by

or

$$p^{2}+m^{2}=0$$

$$|p|^{2}+m^{2}-p_{0}^{2}=0$$

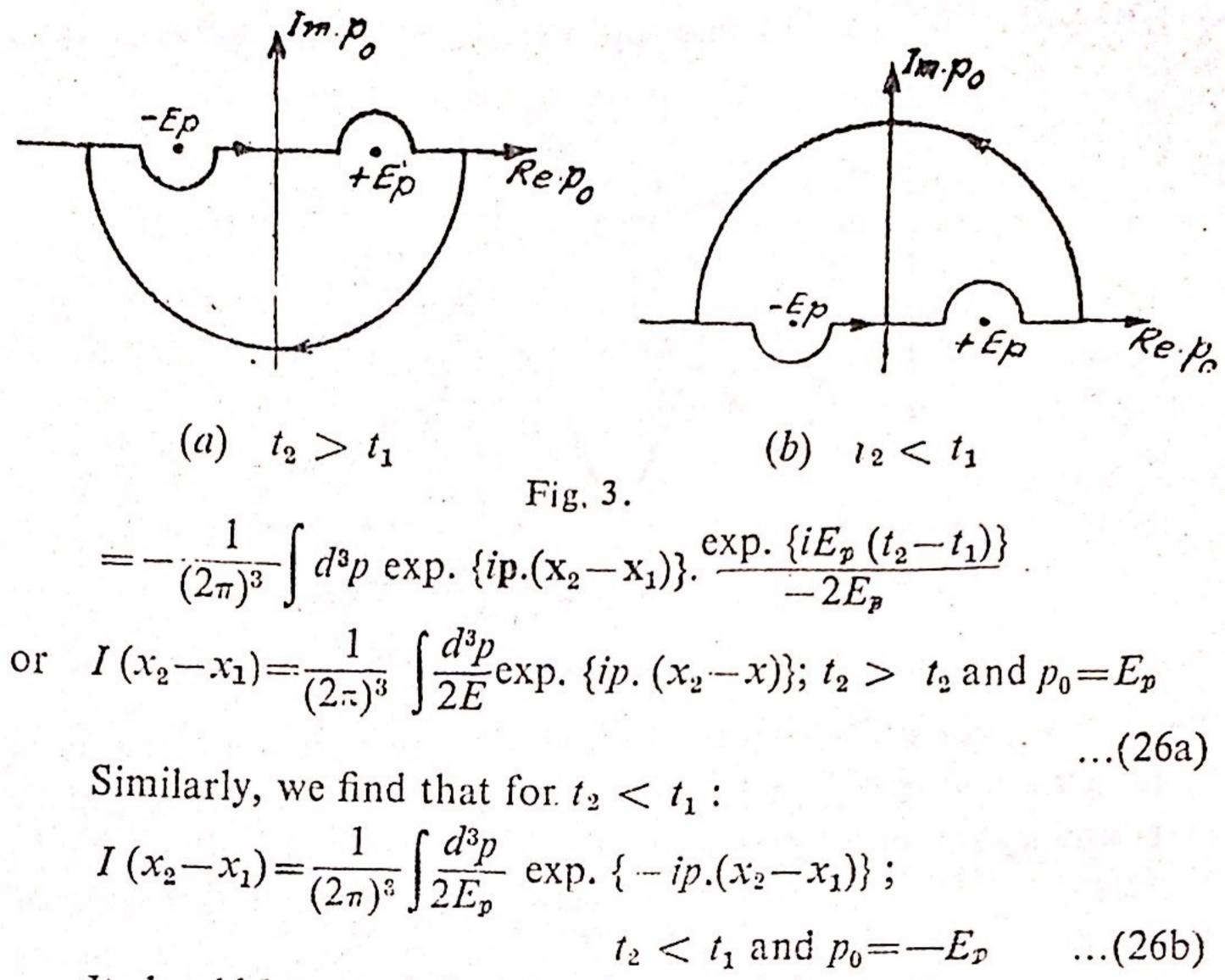
$$|p|^{2}+m^{2}-p_{0}^{2}=0 \Rightarrow p_{0}=\pm E_{p}$$

or To evaluate the integral (22) we first have to make a proper choice of the contour. The contour is determined by the term exp. $\{-ip_0 \ (t_2-t_1)\}$. Since $t_2 > t_1$, due to causality conservation, the contour should be closed from below the real axis and as $t_2 > t_1$ corresponds to the forward motion in time the pole at $p_0 = +E_p$ should be included inside the contour, However, if $t_2 < t_1$, then the contour should be closed from above the real axis and this time the contribution will come from the pole at $p_0 = -E_p$ only, in order to conserve the causality. The two contours are shown in Fig. 3.

Hence by applying the residence theorem, for $t_2 < t_1$, we have

$$I(x_2-x_1) = -2\pi i \cdot \frac{-i}{(2\pi)^4}$$

$$\times \int d^3p \exp(i\mathbf{p} \cdot (\mathbf{x}_2-\mathbf{x}_1)) \cdot \lim_{p_0 \to E_p} \underbrace{\exp(-ip_0 (t_2-t_1)) \cdot (p_0-E_p)}_{E_p^2-p_0^2}$$



It should be noted that the change of sign in the exponential term of the integrand in the above eqns. does not change the value of the integral w.r.t d^3p , since the integration is over the entire momentum space and E_p is an even function of p.

Using (26 a and b) into (23) we get the propagators for the Dirac particles of positive and the negative energies. We see that $K(x_2-x_1)$ is not zero even for $t_2 < t_1$ contrary to the case of Schroedingers nonrelativistic particle. Here, it represents the propagator for a negative energy particle moving backward in time $(t_2 < t_1)$. Feynman interpreted it as the position propagator. The Feynman's theory of position greatly simplifies the interpretation of the processes like pair production and pair annihilation, as explained below:

Let us consider the process of the fig. 4 shown on page 528. It shows an electron originating at x and ending up at x'. Along the way, a pair is produced at the point x_1 ; the positron of the pair annihilates the initial electron at x_3 , the electron of the pair propagates up to x_2 , where it is scattered by some potential and and theory propagates up to x'. Thus we see that it is not the same electron that starts from x, but a different electron from the pair production which reaches at x'. Thus in the Dirac theory, not only we have to consider more than one particle in the process,

but also the trajectory of the particle becomes discontinuous. On the other hand if we take up Feynman's point of view, then

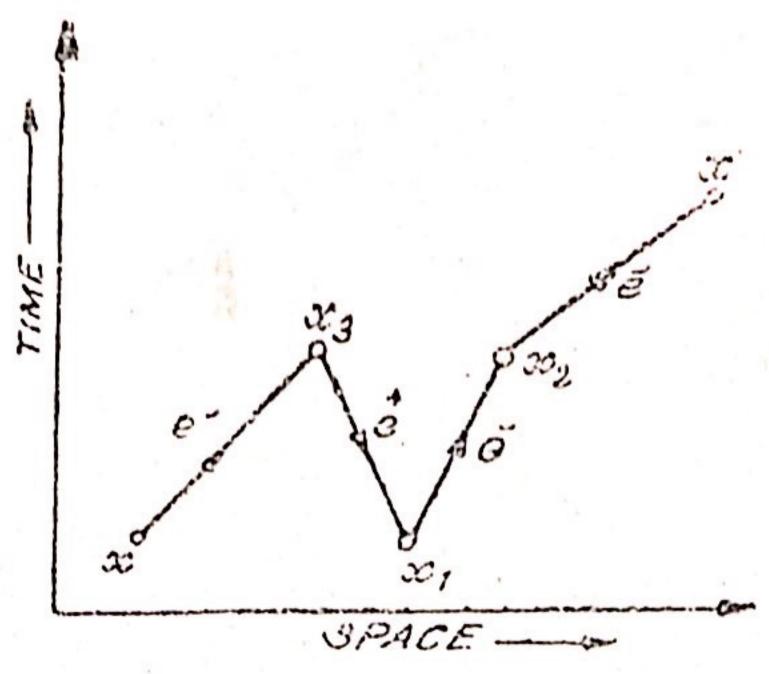


Fig. 4.

the electron travels from x to x_3 forward in time, then it is scattered from x_3 to x_1 as a negative energy state, it again gets scattered at x_1 and x_2 and continues to x'. Hence the same electron reaches x'. Feynman's interpretation restores the one particle nature of Dirac equation. We can now talk of a single negative energy state moving back in time, while in hole theory, we have to consider the entire infinite sea of negative energy states.

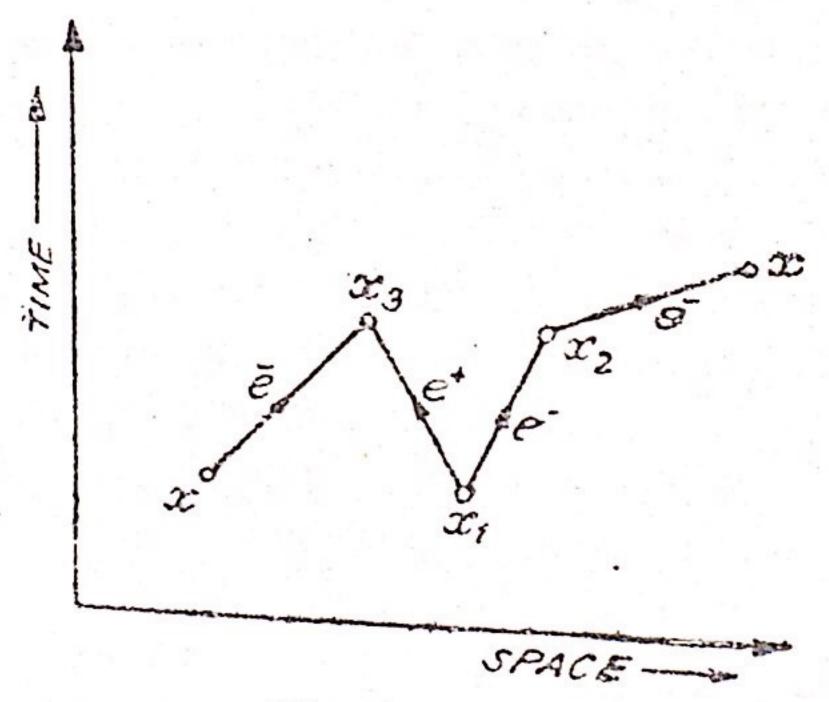


Fig. 5.

11.3. PROPAGATOR FOR A DIRAC ELECTRON INTERACT. ING WITH AN EXTERNAL E.M. FIELD:

We have seen that the free particle propagator K_0 (x_2-x_1) of the Dirac eqn. satisfies the equation:

 $(\partial_2 + m) K_0 (x_2 - x_1) = -i\delta^4 (x_2 - x_1)$ The interacting with field A_{μ} can be incorporated by replacing ∂_{μ} by $(\partial_{\mu} - ieA_{\mu})$. Therefore, for a Dirac equation in external electromagnetic field, the propagator $K(x_2-x_1)$, should satisfy the equation:

$$(\mathcal{Z}_{2}-ieA_{2}+m) K (x_{2}-x_{1}) = -i\delta^{4} (x_{2}-x_{1}) \qquad \dots (28)$$
or
$$(\mathcal{Z}_{2}+m) K (x_{2}-x_{1}) = -i\delta^{4} (x_{2}-x_{1}) + ieA_{2} K (x_{2}-x_{1})$$
or
$$(\mathcal{Z}_{2}+m) K (x_{2}-x_{1}) = -i\delta^{4} (x_{2}-x_{1})$$

$$+ie \int d^{4}x_{3}A_{3} K (x_{3}-x_{1}) \delta^{4} (x_{2}-x_{3}) \dots (29)$$

Also from (27) we can always write

$$K_0(x_2-x_1)=-i(\vartheta_2+m)^{-1}\delta^4(x_2-x_1) \qquad ...(30)$$

Using it in (29) we get:

de

$$K(x_2-x_1) = -i (\mathfrak{F}_2+m)^{-1} \delta^4 (x_2-x_1) + ie \int d^4x_3 A_3 K(x_3-x_1) (\mathfrak{F}_2+m)^{-1} \delta^4 (x_2-x_3)$$

$$=K_0(x_2-x_1)+(-e)\int d^4x_3 K_0(x_2-x_3) A_3 K(x_3-x_1) \dots (31)$$

Eqn. (31) gives an expression for $K(x_2-x_1)$ in terms of the free particle propagator. K_0 . The advantage of this integral equation lies in the fact that in addition to containing all the boundary conditions, it can readily be solved by successive approximations. In the first approximation, we substitute the value of $K(x_3-x_1)$ into the r.h.s. of (31) from the eqn. (31) itself. From (31) we write

(31) We write
$$K(x_3-x_1)=K_0(x_3-x_1)+(-e)\int d^4x_4 K_0(x_3-x_4) A_4 K(x_4-x_1)$$

Now substituting it into (31), we get

Now substituting it into (51), we get
$$K(x_2-x_1)=K_0 (x_2-x_1)$$

$$+(-e) \int d^4x_3 K_0 (x_2-x_3) A_3 [K_0 (x_3-x_1)+(-e) \int d^4x_4$$

$$\times \{(K_0 (x_3-x_4) A_4 K(x_4-x_1)\}]$$

$$=K_0 (x_2-x_1)+(-e) \int d^4x_3 K_0 (x_2-x_3) A_3 K_0 (x_3-x_1)$$

$$+(-e)^2 \iint d^4x_3 d^4x_4 K_0 (x_2-x_3) A_3 K_0 (x_3-x_4) A_4 K (x_4-x_1)$$

Making successive substitutions like it we get the generalized result:

$$K(x_2-x_1)=K_0(x_2-x_1)+(-e)\int K_0(x_2-x_3) A_3 K_0(x_3-x_1) d^4x_2$$

$$+(-e)^2 \int \int d^4x_3 d^4x_4 K_0(x_2-x_3) A_3 K_0(x_3-x_4) A_4 K_0(x_4-x_1)$$

 $+(-e)^{3} \iiint d^{4}x_{3} d^{4}x_{4} d^{4}x_{5} K_{0} (x_{2}-x_{3}) A_{3} K_{0} (x_{3}-x_{4})$ $\times A_{4} K_{0} (x_{4}-x_{5}) A_{5} K_{0} (x_{5}-x_{1}) + ...$ The lize the various terms

Let us now visualize the various terms of the series for K (x_2) by space time diagrams. The first term ' x_3 " is the (x_4) to x_4 for a free electron moving from x_4 to x_4 in the fourpropagator al space.

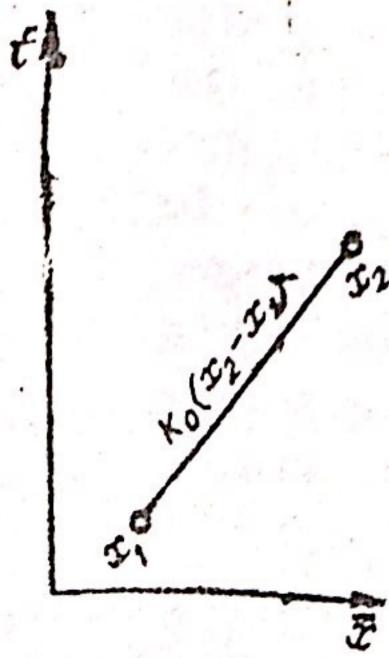


Fig. 6.

The second term shows the propagation of the particle from x_1 to x_3 where it suffers an e.m. scattering by a field A_3 . From x_3 it propagates freely to point x_2 in space. Since the point x_3 can be any where in space, we have integrated over all the space w.r.t. x_3 .

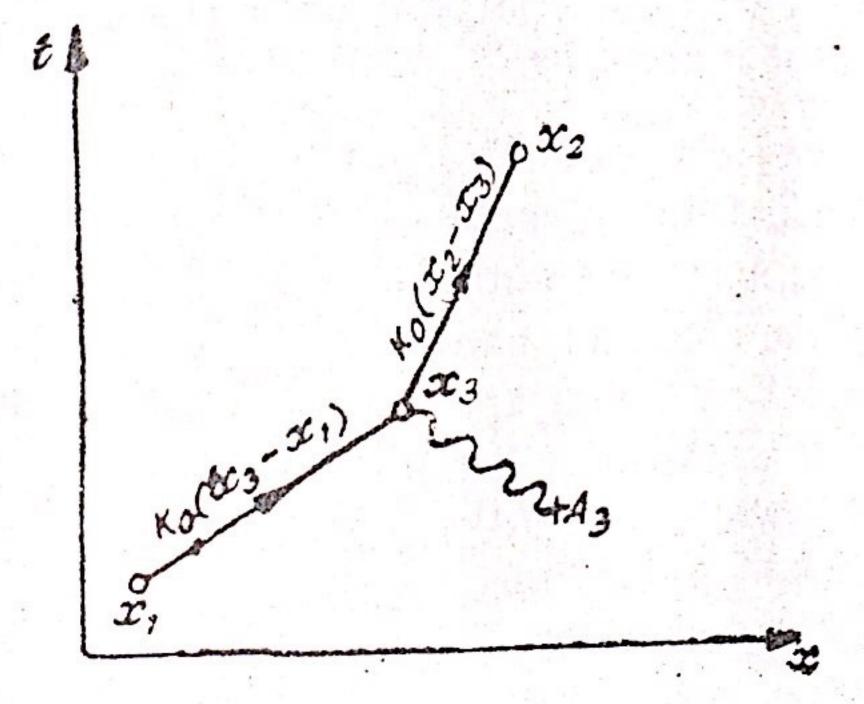


Fig. 7

The third term represents the situation when the electron suffers two scatterings, one at point x_4 by a field A_4 and again at point x_8 by a field A_3 . Here also we integrate over whole of the space w.r.t. x_3 and x_4 , because x_3 and x_4 can lie anywhere in the space.

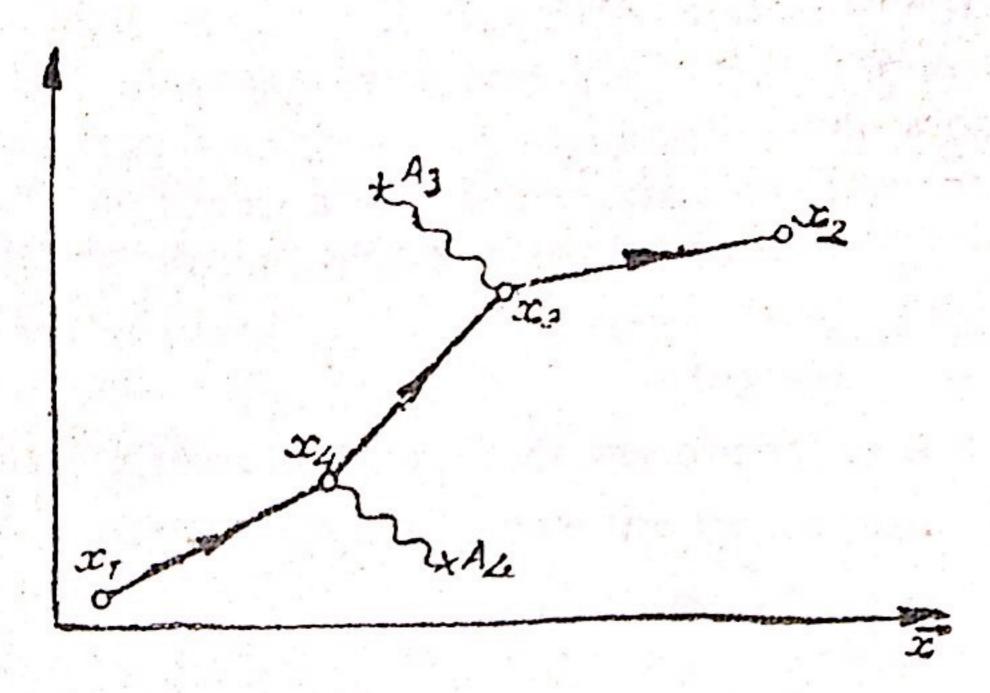


Fig. 8

Similarly, the *n*th term represents the *n*th order scattering of the particle. At the point x_i the particle is scattered with a probability amplitude per unit space time to a new volume to a new wave propagating forward in time with amplitude $K(x_{i+1}-x_i)$. This amplitude is then summed over all space-time points in which the interactions can occur. We may say that the interaction at the *i*th point destroys the particle propagating up to x_i and creates a new particle which propagates on to x_{i+1} with $t_{i+1} \ge t_i$.

11.4. FORMULATION OF SCATTERING THEORY INTERMS OF FEYNMAN'S PROPAGATORS:

We have seen that given an initial state $\psi(x_1)$ of a system at point x_1 and time t_1 ; the final state $\psi(x_2)$ at the point x_2 and at a later time t_2 is given by

$$\psi(x_2) = \int d^3x_1 K(x_2 - x_1) \gamma_4 \psi(x_1) \dots (33)$$

Here $\psi(x_2)$ is a general final state. If we wish to find the probability amplitude of the particle being in a particular final state $\phi_f(x_2)$ from a definite initial state $\phi_t(x_1)$, it will be proportional to the scalar product:

$$\{\phi_f(x_2), \psi(x_2)\} = \left[\phi_f(x_2), \int d^3x_1 K(x_2 - x_1) \gamma_4 \phi_i(x_1) \right]$$

$$= \int d^3x_2 \phi_f^{\dagger}(x_2) \int d^3x_1 K(x_2 - x_1) \gamma_4 \phi_i(x_1) \dots (34)$$

Now the propagator $K(x_2-x_1)$ on the r.h.s. of the above equation can be approximated by the series (32). Let us see the effect of successive approximations in the series (32). Suppose we retain the first or zeroth order term, then $K(x_2-x_1)-K_0$ (x_2-x_1) .

In this case, the final state of the particle won't be different from the initial state, i.e., there won't be any scattering and hence K_0 (x_2-x_1) does not contribute to the transition probability amplitude. The transition matrix element for a transition from the initial state $\phi_1(x_1)$ to the final state $\phi_1(x_2)$, in the zeroth order process vanishes

$$M^{(0)}=0$$
 ...(35)

For the first order process, the transition matrix element is given by

$$M^{(1)} = (-e) \iint d^3x_1 d^3x_2 \phi_f^{\dagger}(x_2)$$

$$\times \int d^4x_3 K_0 (x_2 - x_3) A_3 K_0 (x_3 - x_1) \gamma_4 \phi_i (x_1)$$
or
$$M^{(1)} = (-e) \int d^4x_3 \left\{ \int d^3x_2 \phi_f^{\dagger}(x_2) K_0 (x_2 - x_2) \right\}$$

$$\times A_3 \left\{ \int d^3x_1 K_0 (x_3 - x_1) \gamma_4 \phi_i (x_1) \right\} \dots (36)$$

To simplify it further, we write for the final state ϕ_i (x_3), using equation (33), as

$$\phi_{f}(x_{3}) = \int d^{3}x_{2} K_{0} (x_{3} - x_{2}) \gamma_{4} t_{1} (x_{2})$$

$$\therefore \quad \bar{\phi}_{f}(x_{3}) = \int d^{3}x_{2} \phi_{i}^{\dagger} (x_{2}) \gamma_{4} K_{0}^{\dagger} (x_{3} - x_{2}) \gamma_{4}$$

$$\dots(37)$$
Now,

$$K_{0}(x_{3}-x_{2}) = -\frac{i}{(2\pi)^{4}} \int d^{4}p \exp \{ip.(x_{3}-x_{2})\} \frac{m-ip}{m^{2}+p^{2}}$$

$$= -\frac{i}{(2\pi)^{4}} \int d^{4}p \exp \{ip.(x_{3}-x_{2})\} \frac{m-i}{m^{2}+p^{2}}$$

$$\therefore \gamma_{4} K_{0}^{\dagger}(x_{3}-x_{2}) \gamma_{4} = \frac{i}{(2\pi)^{4}} \int d^{4}p \exp \{-ip.(x_{3}-x_{2})\}$$

$$\times \frac{m-i}{m^{2}+p^{2}}$$

$$= -K_{0}(x_{2}-x_{3})$$

Hence we have

$$\overline{\phi}_{f}(x_{3}) = -\int d^{3}x_{2} \, \phi_{i}^{\dagger}(x_{2}) \, K_{0}(x_{2} - x_{3}) \qquad (38)$$

Using it into (36) we get

$$M^{(1)} = e \int d^4x_3 \, \bar{\phi}_I(x_3) \, A_8 \, \phi_i(x_3) \dots (33)$$

This equation corresponds to an electron in the initial state ϕ_i (x_3) being scattered at the point x_3 by an interaction with the electromagnetic field A_3 and then propagating to the point x_2 in the final state ϕ_i (x_3) . Since the point x_3 can be any where in the space, an integration over whole of the space occurs.

If we consider the second order term, then the transition matrix element will be given by

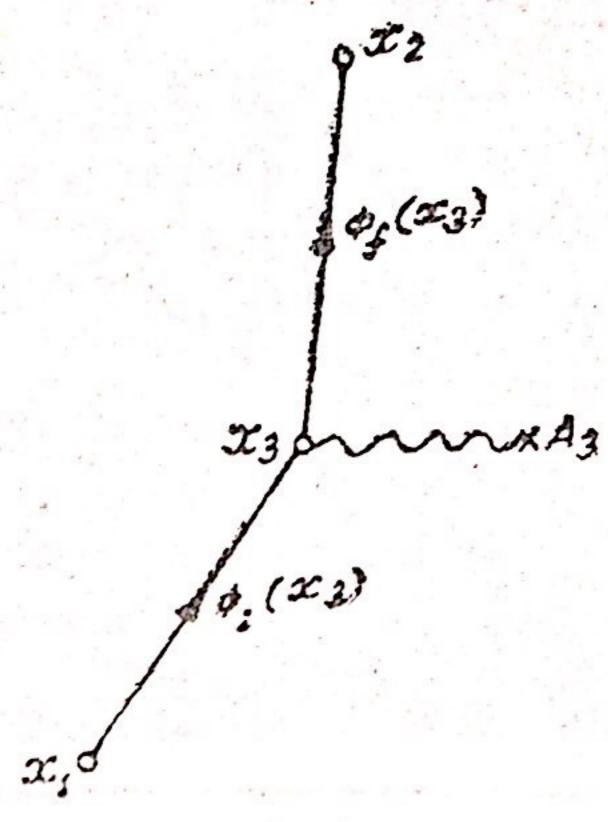


Fig. 9.

$$M^{(2)} = -(-e)^2 \int \int d^4x_3 \ d^4x_4 \ \phi_f(x_3) A_2 K_0 (x_3 - x_4) A_4 \phi_i (x_4) \dots (40)$$

$$M^{(2)} = -(-e)^2 \int \int d^4x_3 \ d^4x_4 \ \phi_f(x_3) A_2 K_0 (x_3 - x_4) A_4 \phi_i (x_4) \dots (40)$$

This expression corresponds to x_1 double scattering of the initial state ϕ_i (x_4) at the points x_4 and x_3 into the final state ϕ_i (x_3). (See fig. 8)

11.5. RUTHERFORD'S SCATTERING OF AN ELECTRON FROM A FIXED COULOMB POTENTIAL:

If p is the momentum of the electron in the initial state ϕ_i and if p' is its momentum in the final state ϕ_i after interaction with an electromagnetic potential A(x), then the first order transition matrix element is given by

$$M^{(1)} = e \int d^4x \, \overline{\phi}_f(x) \, A(x) \, \phi_i(x)$$
 ...(41)

In the initial and in the final states, the electron is at asymptotic distances from the potential and hence the interaction with the potential can be neglected. We can approximate these states by the following normalized plane wave solutions of the Dirac equation;

solutions of the Dirac equation,
$$\phi_{i}(x) = \sqrt{\left(\frac{m}{E_{p}V}\right)} u^{r}(\mathbf{p}) \exp_{i}\left\{ip.x\right\}}$$
Fig. 10.
and
$$\phi_{i}(x) = \sqrt{\left(\frac{m}{E_{p}'V}\right)} u^{r}(\mathbf{p}') \exp_{i}\left\{ip'.x\right\}}$$
...(42)

$$M^{(1)} = \frac{e}{V} \cdot \sqrt{\left(\frac{m^2}{E'_p E_p}\right)} \cdot \int_u^{-r'} (\mathbf{p}') \exp. \quad \{-ip'.x\} \land (x)u^r (\mathbf{p}) \times \exp. \quad \{ip.x\} \ d'x \}$$

$$= \frac{e}{V} \cdot \sqrt{\left(\frac{m^2}{E_p E_{p'}}\right)} \cdot u^{-r'}(p') \int \exp \{i (p-p').x\}$$

$$\times A (x) d^4x u^r (p)$$

$$= \frac{e}{V} \cdot \sqrt{\left(\frac{m^2}{E_p E_{p'}}\right)} \cdot u^{-r'}(p) \int \exp \{iq.x\}$$

$$\times (A (x) d^4x u^r (p); \text{ with } q=p-p'$$

$$= \frac{e}{V} \sqrt{\left(\frac{m^2}{E_p E_{p'}}\right)} \cdot u^{-r'}(p') A (q) u^r (p), \dots (43)$$

where $A(q) = \int \exp \{iq.x\} A(x) d^4x$,

is the Fourier Transform of A(x). Now the static Coulomb potential is given by:

$$A(x)=0, A_4(x)=\frac{ieZ}{r}$$
 ...(44)

where Z is the number of protons in the scattering nucleus. Hence we have

$$A(q) = ieZ \int \exp \{iq.x\} \frac{\gamma_4}{r} d^3r dt$$
 ...(45)

First we calculate the space part of the integral in (45):

$$ieZ \int \exp. \{iq.r\} \frac{\gamma_4}{r} d^3r = ieZ \gamma_4 \int_0^{2\pi} d\rho \int_0^{\infty} \frac{r^2 dr}{r}$$

$$\times \int_0^{\pi} \exp. \{i \mid q \mid r \cos \theta\} \sin \theta d\theta$$

$$= ieZ \gamma_4.2\pi. \int_0^{\infty} r dr \left[\frac{\exp. \{i \mid q \mid rx\}}{i \mid q \mid r} \right]_{x=-1}^{+1}$$

$$= ieZ \gamma_4.2\pi. \int_0^{\infty} \frac{dr}{\mid q \mid} .2 \sin \left(\mid q \mid r\right)$$

$$= ieZ \gamma_4.4\pi. \int_0^{\infty} \frac{\sin \mid q \mid r}{\mid q \mid} dr$$

Now,
$$\int_{0}^{\infty} \frac{\sin |\mathbf{q}| r}{|\mathbf{q}|} dr = \frac{1}{|\mathbf{q}|} \int_{0}^{\infty} \sin x \frac{dx}{|\mathbf{q}|} = \frac{1}{|\mathbf{q}|^{2}} Im. \int_{0}^{\infty} \exp\{ix\} dx$$

does not exist because the integrand is oscillatory. Hence, to evaluate it, we play a simple trick that we add a converging factor exp. $\{-i\xi x\}$ to the integrand and later on take the limit $\xi \rightarrow 0$. Thus

Im.
$$\int_{0}^{\infty} \exp \{ix\} dx = Im \left(\lim_{\xi \to 0} \int_{0}^{\infty} \exp \{-i(\xi - 1) x\} dx\right) = 1$$
.
 $\therefore ieZ \int \exp \{iq.r\} \frac{\gamma_4}{r} d^3r = \frac{4\pi ieZ\gamma_4}{|q|^2}$...(46)

For the time part of the integral in eqn. (45) we have:

$$\int_{-\infty}^{+\infty} \exp\left\{-iq_0 t\right\} dt = 2\pi \, \delta \, (q_0) = 2\pi \delta \, (E_p - E_{p'}) = 2\pi \delta(0) \, \dots (47)$$

Because $E_p = E_p'$ for an elastic scattering.

Now
$$2\pi\delta (E_p - E_{p'}) = \lim_{T \to \infty} \int_{-T/2}^{T/2} \exp \left\{-i (E_p - E_{p'}) t\right\} dt$$

Hence,
$$2\pi\delta(0) = \lim_{T \to \infty} \int_{-T/2}^{T/2} dt = T$$
 ...(48)

Here T is the total time in which the transition takes place. So we get:

$$\int_{-\infty}^{+\infty} \exp\left\{-iq_0t\right\} dt = T \qquad ...(49)$$

From (46) and (49) we obtain the integral (45) as:

$$A(q) = \frac{4\pi \ ieZ}{|q|^2} \frac{\gamma_4}{r} . T \qquad ...(50)$$

Therefore,

$$M^{(1)} = \frac{4\pi Te}{V} \frac{m}{\sqrt{(E_p E_p')}} \cdot \bar{u}^{r'} (p') \left(\frac{ieZ}{|q|^2}\right) \gamma_4 u^r (p) \qquad ...(51)$$

From it we can get the transition probability $|M^{(1)}|^2$. Now the final state is not a sharply defined one. It is a group of states, because the direction of the three-dimensional momentum changes. To take it into account we should sum over all the final states and hence the transition probability summed over all the final states will be given by:

$$\Sigma \mid M^{(1)} \mid^2$$
 final ... (52) states

Thus the transition probability per unit time can be written as:

$$w = \frac{1}{T} \cdot \Sigma |M^{(1)}|^2 = \Sigma |\overline{M}|^2 \cdot 2\pi \delta (q_0), \dots (53)$$
final final

states states

where
$$\overline{M} = \frac{4\pi e}{V} \frac{m}{\sqrt{(E_p E_{p'})}} \cdot u^{-r'}(p') \left(\frac{ieZ}{|q|^2}\right) \gamma_4 u^r (p) ... (54)$$

In writing eqn. (53) we have used

$$T^2 = [2\pi \delta (q_0)]^2 = T.2\pi \delta (q_0),$$

which is perfectly justified for long $T(T\rightarrow\infty)$. Changing the summation on the r.h.s. of (53) into integration, we can write

$$w = \int |\overline{M}|^2 2\pi \delta (p_0 - p_0') \cdot \frac{V}{(2-)^3} |\mathbf{p'}|^2 dp' d\Omega'$$

$$= \frac{V}{(2\pi)^2} \int |\overline{M}|^2 \, \delta \, (E_p - E_{p'}) \, |\mathbf{p'}|^2 \, dp' \, d\Omega'$$

Hence the transition probability per unit time per unit solid angle is given by

$$\frac{\delta w}{\delta \Omega'} = \frac{V}{(2\pi)^2} \int ||\overline{M}||^2 \, \delta \, (E_p - E_{p'}) \, ||\mathbf{p}'||^2 \, dp'
= \frac{V}{(2\pi)^2} \int ||\overline{M}||^2 \, ||\mathbf{p}'||^2 \left(\frac{dp'}{dE_{p'}}\right) \delta \, (E_p - E_{p'}) \, dEp'
= \frac{V}{(2\pi)^2} \, ||\overline{M}||^2 \, ||\mathbf{p}'||^2 \left(\frac{dp'}{dE_{p'}}\right) E_{p'} = E_p \qquad ...(55)$$

We have evaluated the above integral by using the property of Dirac delta function $\delta (E_p - E_{p'})$.

Now,

$$E^{2}_{p'} = |\mathbf{p'}|^{2} + m^{2}$$

$$\therefore 2E_{p'} dE_{p'} = 2 |\mathbf{p'}| d|\mathbf{p'}|$$

$$\Rightarrow \left(\frac{dp'}{dE_{p'}}\right) = \frac{E_{p'}}{|\mathbf{p'}|} \text{ and } \left(\frac{dp'}{dE_{p'}}\right) E_{p'} = E_{p} = \frac{E_{p}}{|\mathbf{p'}|}$$

Hence we have

$$\frac{\delta w}{d\Omega'} = \frac{V}{(2\pi)^2} |\overline{M}|^2 |p'| E_p \qquad ...(56)$$

Since the incident beam of electrons is unpolarized and it is not possible to fix the spin of the electron in the final state, we average over the spin of the final electron and sum over the initial electron spin states:

$$\frac{\delta w}{\delta \Omega'} = \frac{1}{2} \sum_{r} |\overline{M}|^{2} \cdot \frac{V |p'|}{4\pi^{2}} E_{p}$$

$$= \frac{1}{2} \sum_{r} |u^{-r'}(p') \gamma_{4} u'(p)|^{2} \cdot \left(\frac{4\pi e}{V}\right)^{2} \cdot \frac{m^{2}}{E_{p}E_{p'}}$$

$$\times \left(\frac{eZ}{|q|^{2}}\right)^{2} \cdot \frac{V |p'| \cdot E_{p}}{4\pi^{2}} ... (57)$$

Now,

$$\frac{1}{2} \sum_{r} \sum_{r'} |u^{-r'}(p') \gamma_4 u^{r'}(p)|^2 = \frac{1}{2} T_r \left[\gamma_4 \Lambda^{(+)}(p) \gamma_4 \Lambda^{(+)}(p') \right] \\
= \frac{1}{8m^2} T_r \left[\gamma_4 (m - ip) \gamma_4 (m - ip') \right]$$

$$= \frac{1}{8m^2} \left[m^2 T_r (\gamma_4^2) - T_r (\gamma_4 p \gamma_4 p') \right] \qquad \dots (58)$$

the trace of the product of an odd number of gamma matrices vanishes.}

We have $T_r(\gamma_a^2)=4$, and

$$T_{r} (\gamma_{4} p \gamma_{4} p') = (p_{\mu}p_{\nu}') T_{r} (\gamma_{1}\gamma_{\mu}\gamma_{4}\gamma_{\nu})$$

$$= (p_{\mu}p_{\nu}')(4\delta_{4\mu}\delta_{\nu4} + 4\delta_{4\nu}\delta_{\mu4} - 4\delta_{\mu\nu})$$

$$= 4 (2p_{4}p_{4}' - p_{\mu}p_{\mu}') = -4 (p.p' + E_{p}E_{p}')$$

$$\therefore \frac{1}{2} \sum_{r} \sum_{r'} |u^{-r'}(p') \gamma_{4} u'(p)|^{2} = \frac{1}{2m^{2}} [m^{2} + p.p' + E_{p}E_{p}']$$

$$= \frac{1}{2m^{2}} [m^{2} + |p|^{2} \cos \theta + E_{p}'] \qquad ...(59)$$

 $\{: |p| = |p'| \text{ and } E_p = E_{p'} \text{ for the elastic scattering}\}.$

Here θ is the angle of scattering.

Using $m^2 = E_p^2 - |\mathbf{p}|^2$ into (59) we write:

$$\frac{1}{2}\sum_{r'} |u^{-r'}(\mathbf{p}') \gamma_4 u^r(\mathbf{p})|^2 = \frac{1}{2m^2} \left[2E_p^2 - |\mathbf{p}|^2 + |\mathbf{p}|^2 \cos \theta \right]$$

$$= \frac{2E_p^2}{2m^2} \left[1 - \frac{|\mathbf{p}|^2}{E_p^2} \sin^2 \frac{\theta}{2} \right]$$

$$= \frac{E^2_p}{m^2} \left[1 - v^2 \sin^2 \frac{\theta}{2} \right]$$

$$\{ : v = \frac{|\mathbf{p}|}{E_p} \}$$

Hence we can write (57) as

$$\frac{\delta w}{\delta \Omega'} = \frac{E_{p}^{2}}{m^{2}} \left[1 - v^{2} \sin^{2} \frac{\theta}{2} \right] \cdot \left(\frac{4 \cdot e}{V} \right)^{2} \cdot \frac{m^{2}}{E_{p} E_{p'}} \cdot \left(\frac{eZ}{|\mathbf{q}|^{2}} \right)^{2} \frac{V |\mathbf{p'}|}{4n^{2}} \cdot E_{p}$$

$$= \frac{4e^{4}Z^{2} E_{p} |\mathbf{p}|}{|\mathbf{q}|^{4} \cdot V} \left(1 - v^{2} \sin^{2} \frac{\theta}{2} \right) \qquad ...(60)$$

$$\{ :: E_{p} = E_{p'} & \& |\mathbf{p}| = |\mathbf{p'}| \}$$

Form (60) we can get the differential scattering cross-section by dividing it with the incident flux. Now,

Incident Flux=Density × Velocity

1

$$= \frac{1}{V} \cdot v = \frac{1}{V} \cdot \frac{|\mathbf{p}|}{E_n}$$

$$\frac{d\sigma}{d\Omega} = \frac{\delta w}{d\Omega} / \text{Incident Flux}$$

$$= \frac{4Z^2 e^4}{|\mathbf{q}|^4} E_{p^2} \left(1 - v^2 \sin^2 \frac{\theta}{2} \right)$$

Now,
$$q=p-p'$$

 $\therefore |q|^2=|p|^2+|p'|^2-2p \cdot p'$
 $=2|p|^2-2|p|^2\cos\theta$
 $=4|p|^2\sin^2\theta/2$

Hence, we have

$$\frac{d\sigma}{d\Omega} = \frac{4Z^{2}e^{4}}{16 |\mathbf{p}|^{4} \sin^{4} \theta/2} E_{p^{2}} \cdot \left(1 - v^{2} \sin^{2} \frac{\theta}{2}\right)
\frac{d\sigma}{d\Omega} = \frac{Z^{2}e^{1}}{4v^{2} |\mathbf{p}|^{2}} \cdot \frac{(1 - v^{2} \sin^{2} \theta/2)}{\sin^{4} \theta/2} \dots (62)$$

or

In the limit when $v \to 0$, this formula reduces to the famous Rutherford's formula:

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} \frac{Z^2 e^4}{m^2 v^4} \cdot \frac{1}{\sin^4 \theta/2} \qquad ...(63)$$

Formula (62) is known as Mott's Scattering formula. In the first order approximation, the positron scattering from a fixed Coulomb potential will be identical to that for the electron. However, in the second order calculations, there will be two terms A_3 and A_4 and the interference between these will give rise to a change of sign in case of positron. Thus the two particles will be distinguished.

11.6. ELECTRON SCATTERING FROM A DIRAC PROTON:

In the preceding section we considered the scattering of an electron from a static Coulomb potential. Now we consider the scattering of the electron from the field of a moving proton. The matrix element in the first order approximation is given by

$$M^{(1)} = e \int \overline{\phi}_f(x) A_{\mu}(x) \phi_i(x) d^4x, \qquad ...(64)$$

where $A_{\mu}(x)$ is the em. field due to the moving proton, at the site of the electron. It is governed by the Maxwell's equation

$$\square A_{\mu} = -j_{\mu}. \qquad ... (65)$$

where $j_{\mu}(x)$ is the proton current. Knowing it, we can solve (65) to get $A_{\mu}(x)$. Treating the proton as a point charge, the expression for the current can be written an-

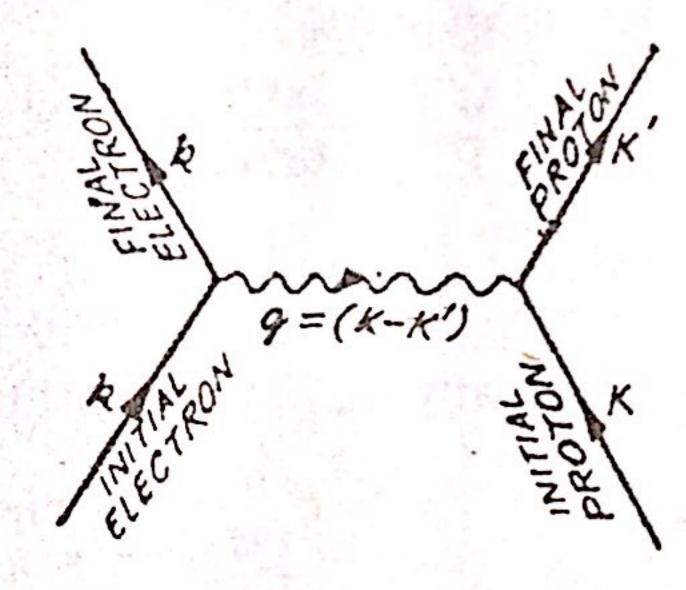


Fig. 11.

alogous to that for the electron as: $\bar{\psi}\gamma_{\mu}\psi$. However, the proton has an extended charge distribution, and if the charge density is P(r), the total charge is given by

$$Ze = \int \rho(\mathbf{r}) d^3r \qquad \dots (66)$$

and the potential $A_{\mu}(x)$ is, therefore defined by:

A
$$(x)=0$$
; $A_0(x)=i\frac{eZ}{r}=i\int \frac{\rho(r)}{r} d^3r$.

The Fourier transform A(q) of A(x) is given by:

$$A(q) = \int d^{4}x \ A(x) \ e^{iq \cdot x} = \int d^{3}r \ dt \ \exp. \ (i\mathbf{q} \cdot \mathbf{r}) \cdot \exp. (-iq_{0}t) \ A_{0}(x)$$

$$= 2\pi \delta(q_{0}) \int d^{3}r \cdot i \int \frac{d^{3}r' \ \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \exp. \ (i\mathbf{q} \cdot \mathbf{r})$$

$$= 2\pi i \ \delta(q_{0}) \int d^{3}r' \ \exp. \ (i\mathbf{q} \cdot \mathbf{r}') \ \rho(\mathbf{r}') \int d^{3}r \frac{\exp. \ [i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')]}{|\mathbf{r} - \mathbf{r}'|}$$

$$= 2\pi i \ \delta(q_{0}) \ Ze \ F(|\mathbf{q}|^{2}) \cdot \frac{4\pi}{|\mathbf{q}|^{2}}, \qquad \dots (67)$$

where, $Ze F(|q|^2) = \int \rho(\mathbf{r}') \exp(i\mathbf{q} \cdot \mathbf{r}') d^3r'$ and the function $F(|\mathbf{q}|^2)$ is called the 'form factor'. For a point change, $\mathbf{q} = 0$ and hence

$$Ze\ F(0) = \int \rho\ (\mathbf{r}')\ \exp\ (i\mathbf{q}\cdot\mathbf{r}')\ d^3r' = Ze \Rightarrow F(0) = 1.$$

For an extended charge, the distribution of charge is contained in $F(|\mathbf{q}|^2)$. Hence the proton current, corrected for the distribution of its charge, can be written as

$$j_{\mu} = ie\psi\gamma_{\mu} \psi F(\mid \mathbf{q}^{2}) \qquad ...(68)$$

However, for the sake of simplicity, we shall ignore the structure of the proton and take $F(|q|^2)=1$. Due to the motion of the proton, there is associated a magnetic energy $-\mu.B$. where μ is the magnetic dipole moment of the proton. We also ignore the contribution due to it in the current density. Hence we can write the expression for the current in the momentum space as

$$j_{\mu}(x) = \frac{1}{V} \sqrt{\left(\frac{M^2}{E_K E_{K'}}\right)} \cdot [i.e. \, \bar{u}(K') \, \gamma_{\mu} \, u(K) \, e^{iq \cdot x}]$$

$$= j_{\mu}(q) \, e^{iq \, x}, \text{ where } j_{\mu}(q) = \frac{1}{V} \sqrt{\left(\frac{M^2}{E_K E_{K'}}\right)}$$

$$\times ie\bar{u}(K') \, \gamma_{\mu} \, u(K) \qquad \dots (69)$$

Substituting it into (65), we have

Using it into (64), we obtain:

$$M^{(1)} = \frac{1}{V} \cdot \sqrt{\left(\frac{m^2}{E_k E_{k'}}\right)} \cdot e\bar{u}(\mathbf{k'}) \, \gamma_{\mu} \, u(\mathbf{k})$$

$$\times \int d^4 x \, \exp \left[i \, (k-k') \cdot x\right] \frac{j_{\mu} \, (q)}{q^2} \cdot e^{jq \cdot x}$$

$$= \frac{e}{V} \cdot \sqrt{\left(\frac{m^2}{E_k E_{k'}}\right)} \cdot \bar{u}(\mathbf{k'}) \, \gamma_{\mu} \, u(\mathbf{k}) \frac{j_{\mu} \, (q)}{q^2}$$

$$\times (2\pi)^4 \, \delta^4 \, (k-k'+K-K') \, \sqrt{\left(\frac{m^2}{E_k E_{k'}}\right)}$$

$$\times \sqrt{\left(\frac{M^2}{E_K E_{k'}}\right)} \cdot \bar{u}(\mathbf{k'}) \, \gamma_{\mu} \, u(\mathbf{k}) \, \frac{1}{q^2} \, \bar{u}(K') \, \gamma_{\mu} \, u(K) \quad \dots (71)$$

$$\{ \because q = K - K' \}$$

$$= (2\pi)^4 \, \delta^4 \, (k-k'+K-K') \, \sqrt{\left(\frac{m^2}{E_k E_{k'}}\right)}$$

$$\times \sqrt{\left(\frac{M^2}{E_k E_{k'}}\right)} \cdot \frac{1}{V^2} \cdot \frac{M}{M},$$
with $\bar{M} = ie^2 \bar{u} \, (\mathbf{k'}) \, \gamma_{\mu} \, u(\mathbf{k}) \, \frac{1}{q^2} \, \bar{u}(K') \, \gamma_{\mu} \, u(K) \quad \dots (72)$

Hence the transition probability per unit time summed over all the final states is given by

$$w = \frac{1}{T} \cdot \sum_{i=1}^{\infty} |M^{(i)}|^2$$
finial
states

For one dimension we have $2\pi\delta$ $(q_0)=T$. Hence in four dimensions, to include the space as well as time interval, we have

$$(2\pi)^{\epsilon} \delta^{\epsilon} (k-k'+K-K') = TV, \qquad ...(73)$$

where T is the total time of transition and V is the volume of normalization, Therefore,

$$w = \frac{1}{T} \sum_{\substack{k = 1 \ \text{final} \\ \text{states}}} |\bar{M}|^2 \cdot VT. (2\pi)^4 \delta^4 (k - k' + K - K') \cdot \frac{1}{V^4}$$

$$\times \frac{m^2}{E_k E_{k'}} \cdot \frac{M^2}{E_K E_{K'}} \qquad \dots (74)$$

Now the number of final states of a specified spin in the momentum interval d^3K' d^3k' is given by

$$V \cdot \frac{d^3 K'}{(2\pi)^3} V \cdot \frac{d^3 k'}{(2\pi)^3} \dots (75)$$

Hence we have

W=
$$\sum_{|\vec{M}|^2} |\vec{N}|^2 \cdot V \, \delta^4 \, (K+k-K'-k') \, (2\pi)^4 \cdot \frac{1}{V^4} \frac{m^2 M^2}{E_k E_{k'} E_K E_{K'}}$$

final $\times V \, \frac{d^3 k'}{(2\pi)^3} \cdot V \, \frac{d^3 K'}{(2\pi)^3}$.

Changing the summation in the above into integration,

Changing the summation
$$W = \iint \frac{|\overline{M}|^2}{|V|} \cdot \frac{m^2 M^2}{E_k E_k' E_k E_{K'}} \cdot \frac{1}{(2\pi)^2} \delta^4 (K + k - K' - k') d^3 K' d^3 k' d\Omega'$$

$$\frac{\delta w}{\delta \Omega'} = \frac{|\overline{M}|^2}{V} \cdot \frac{m^2 M^2}{E_k E_{k'} E_{K} E_{K'}} \cdot \frac{1}{(2\pi)^2} \cdot \int \delta \left(K_0 + k_0 - K_0' - k_0' \right) d^3 \mathbf{k'} \\
= \frac{|\overline{M}|^2}{V} \cdot \frac{m^2 M^2}{E_k E_{k'} E_{K} E_{K'}} \cdot \frac{|\mathbf{k'}|^2}{(2\pi)^2} \int \delta \left(K_0 + k_0 - K_0' - k_0' \right) d |\mathbf{k'}| \\
\dots (76)$$

Now,

$$\int \mathcal{E}(K_{0}+k_{0}-K_{0}'-k_{0}') d | \mathbf{k}' |
= \int \mathcal{E}[K_{J}+k_{0}-\sqrt{(m^{2}+|\mathbf{k}'|^{2})}-\sqrt{(M^{2}+|\mathbf{K}'|^{2})}] d | \mathbf{k}' |
= \frac{d | \mathbf{k}' |}{d [\sqrt{(m^{2}+|\mathbf{k}'|^{2})}+\sqrt{(M^{2}+|\mathbf{K}'|^{2})}]}
= \int \mathcal{E}[K_{J}'+K_{J}'] dx \mathcal{E}[K_{J}'] dx \mathcal{E}[K_{$$

Hence we have,

$$\frac{\delta w}{\delta \Omega'} = \frac{|M|^2}{V} \cdot \frac{m^2 M^2}{E_k E_{k'}} \cdot \frac{1}{(2\pi)^2} \cdot \frac{E_{k'} E_{K'}}{|k'|} \cdot \frac{E_{k'} E_{K'}}{(E_{K'} + E_{k'})} \cdot \frac{1}{|k'|} = \frac{1}{4\pi^2} |M|^2 \frac{|k'|}{V} \cdot \frac{m^2 M^2}{E_k E_{K'}} \cdot (E_{K'} + E_{k'}) \qquad ...(77)$$

Eventually we have the scattering cross-section,

$$\frac{d\sigma}{d\Omega} = \frac{\delta w}{\delta \Omega'} / \text{Incident Flux.} \qquad ...(78)$$

In the centre of mass system, if an electron and a proton approaches each other with flux $\frac{1}{V} \cdot \frac{|\mathbf{k}|}{E_k}$ and $\frac{1}{V} \cdot \frac{|\mathbf{K}|}{E_K}$, respectively, then the relative flux is given by:

$$\left| \frac{1}{V} \left(\frac{|\mathbf{k}|}{E_{k}} - \frac{|\mathbf{K}|}{E_{K}} \right) \right| = \frac{|\mathbf{k}|E_{K} - \mathbf{K}|E_{k}|}{V|E_{k}E_{K}|}$$

$$\therefore \frac{d\sigma}{d\Omega} = \frac{1}{4\pi^{2}} \cdot |\overline{M}|^{2} \cdot \frac{|\mathbf{k}'|}{V} \frac{m^{2}M^{2}}{E_{k}E_{K}} \cdot \frac{V|E_{k}E_{K}|}{(E_{k}' + E_{K}') |\mathbf{k}|E_{K}|} \cdot \frac{\mathbf{K}|E_{k}|}{E_{k}|}$$

$$= \frac{1}{4\pi^{2}} |\overline{M}|^{2} \cdot |\mathbf{k}'| \frac{m^{2}M^{2}}{(E_{k}' + E_{K}') |\mathbf{k}|E_{K} - \mathbf{K}|E_{k}|} \dots (79)$$
Now, $|\mathbf{k}|E_{K} - \mathbf{K}|E_{k}| = |\mathbf{k}|K_{0} - \mathbf{K}|K_{0}|$

Now,
$$|\mathbf{k} E_K - \mathbf{K} E_k| = |\mathbf{k} K_0 - \mathbf{K} k_0|$$

= $\sqrt{\{(\mathbf{k} K_0 - \mathbf{K} k_0)^2\}}$
= $\sqrt{\{-\frac{1}{2}(k_{\mu}K_{\nu} - K_{\mu}k_{\nu})^2\}}$.

{: the spatial coordinates do not contribute in the centre of mass system of coordinates}

Hence,

$$\frac{d\sigma}{a\Omega} = \frac{1}{4\pi^2} |\vec{M}|^2 \frac{|\mathbf{k}'| m^2 M^2}{(E_{k'} + E_{K'})} \cdot \frac{1}{\sqrt{\{-\frac{1}{2} (k_{\mu} K_{\nu} - K_{\mu} k_{\nu})^2\}}} \\
= \frac{1}{4\pi^2} |\vec{M}|^2 \frac{|\mathbf{k}| m^2 M^2}{(E_{k} + E_{K})} \cdot \frac{1}{\sqrt{\{-\frac{1}{2} (k_{\mu} K_{\nu} - K_{\mu} k_{\nu})^2\}}}, \dots (80)$$

Because $|\mathbf{k}| = |\mathbf{k}'|$, $E_k = E_{k'}$, and $E_K = E_{K'}$ for the elastic scattering.

Formula (80) is called the Moller's invariant cross section. The above treatment is, however, not exact, since we have neglected the proton's structure and its magnetic moment.

11.7. COMPTON SCATTERING:

Second order elastic scattering of electromagnetic radiation from an electron is known as the compton scattering. The transition matrix element for this process is given by:

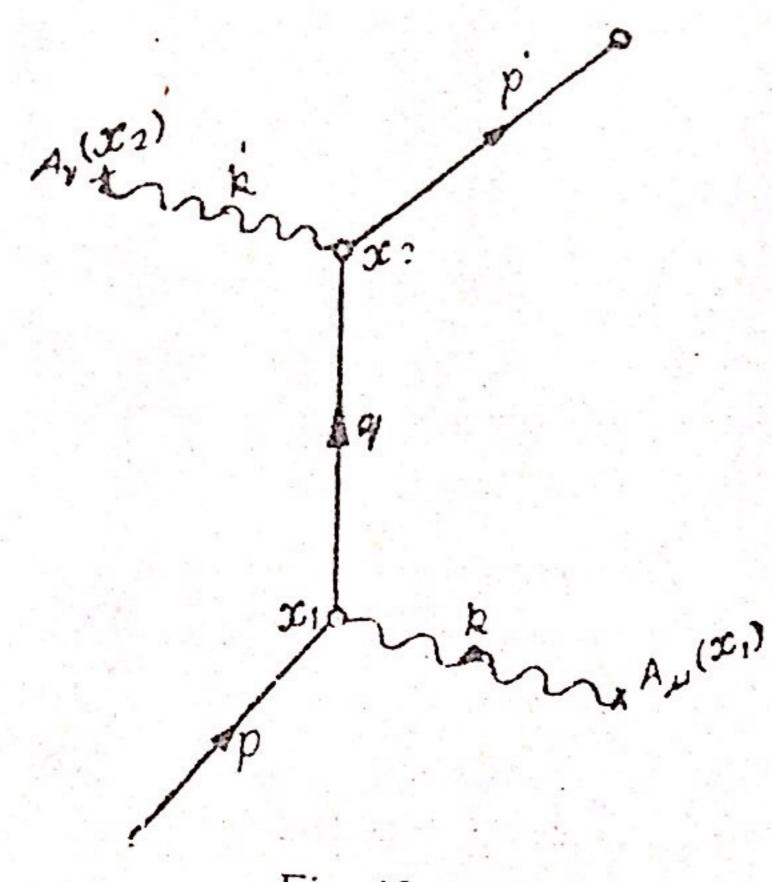


Fig. 12.

$$M^{(2)} = -(-e)^{2} \int d^{4}x_{2} \int d^{4}x_{1} \, \overline{\psi}_{f}(x_{2}) \, A_{v}(x_{2}) \, K_{0}(x_{2}-x_{1})$$

$$A_{\mu}(x_{1}) \, \phi_{I}(x_{1})$$
or
$$M^{(2)} = -e^{3} \int d^{4}x_{2} \int d^{4}x_{1} \, \frac{1}{V} \sqrt{\left(\frac{m^{2}}{E_{p}E_{p}'}\right)}.$$

$$\times \overline{u}^{r'}(p') \, A_{v}(x_{2}) \, K_{0}(x_{2}-x_{1}) \, A_{\mu}(x_{1}) \, u^{r}(p) \, e^{-ip'.x_{2}+ip.x_{1}}$$

$$= -\frac{e^{2}}{V} \, \sqrt{\left(\frac{m^{2}}{E_{p}E_{p}'}\right)} \cdot \int \int d^{4}x_{2} \, d^{4}x_{1} \, \overline{u}^{r'}(p')$$

$$\times A_{v}(x_{2}) \, K_{0}(x_{2}-x_{1}) \, A_{\mu}(x_{1}) \, u^{r}(p) \, e^{-ip'.x_{2}+ip.x_{1}}$$

$$= -\frac{e^{2}}{V} \cdot \sqrt{\left(\frac{m^{2}}{E_{p}E_{p}'}\right)} \cdot \int \int d^{4}x_{2} \, d^{4}x_{1} \, \overline{u}^{r'}(p') \, e^{-ip'.x_{2}+ip.x_{1}}$$

$$= -\frac{i}{(2\pi)^{4}} \int \frac{m-iq}{m^{2}+q^{2}} e^{iq.(x_{2}-x_{1})} \, d^{4}q \times \frac{1}{(2\pi)^{4}} \int e^{ik.x_{1}} \, A_{\mu} \, d^{4}k. u^{r}(p)$$

$$-exp. \, \{-ip'.x_{2}+ip.x_{1}\}$$

$$= \frac{ie^{2}}{V} \cdot \sqrt{\left(\frac{m^{2}}{E_{p}E_{p}'}\right)} \cdot \left[\frac{1}{(2\pi)^{4}}\right]^{3} \cdot \int d^{4}q \, \overline{u}^{r'}(p') \, \frac{m-iq}{m^{2}+q^{2}} \, u^{r}(p)$$

$$\times \int d^{4}k' \, A_{v}(k') \cdot \int d^{4}k \, A_{\mu}(k) \cdot \int d^{4}x_{2} e^{i(q-p'-k').x_{2}}$$

$$\times \int d^{4}x_{1} \, e^{i(p+k-q)}$$

$$= \frac{ie^{2}}{V} \cdot \sqrt{\left(\frac{m^{2}}{E_{p}E_{p}'}\right)} \cdot \frac{1}{(2\pi)^{4}} \int d^{4}q \, \overline{u}^{r'}(p') \, \frac{m-iq}{m^{2}+q^{2}} \, u^{r}(p)$$

$$\times \int d^{4}k' \, A_{v}(k') \cdot \int d^{4}k \, A_{\mu}(k) \cdot \delta^{4}(q-p'-k') \, \delta^{4}(p+k-q)$$

$$= \frac{ie^{2}}{V} \cdot \sqrt{\left(\frac{m^{2}}{E_{p}E_{p}'}\right)} \cdot \frac{1}{(2\pi)^{4}} \int d^{4}q \, \overline{u}^{r'}(p') \, A_{v}(q-p')$$

$$\times \frac{m-iq}{m^{2}+q^{2}} \, A_{\mu}(q-p) \, u^{r}(p') \, A_{v}(q-p')$$

$$\times \frac{m-iq}{m^{2}+q^{2}} \, A_{\mu}(q-p) \, u^{r}(p') \, A_{v}(q-p')$$

$$\dots (81)$$

The topological interpretation of this expression is shown in fig. 12. The initial electron of momentum p absorbs the radiation of momentum k and attains the intermediate state of momentum q. Finally it goes to a state of momentum p' after emitting radiation of momentum k'.

11.8. ELECTRON ELECTRON SCATTERING:

Electron-electron scattering can be handled in a manner very similar to electron proton scattering. However, there is an additional graph arising due to the identity of the electrons. The

Feynman's graphs for this process are shown in Fig. (13). For fig. (13) (a), the first order matrix element is written as.

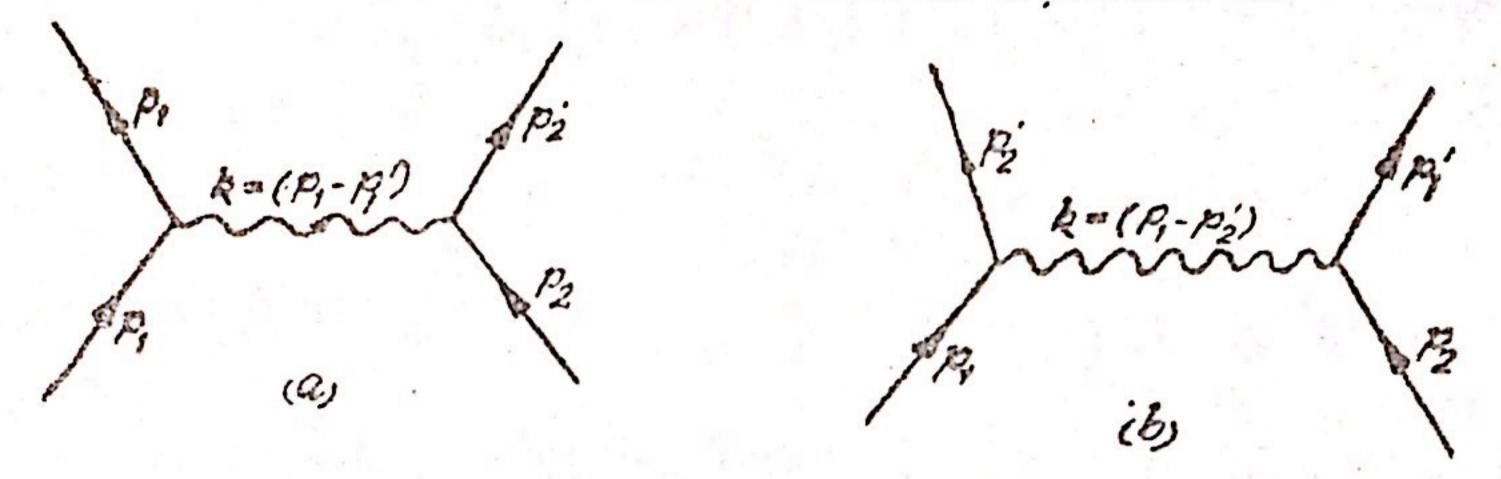


Fig. 13.

$$M^{(1)} = e \int \overline{\phi}_f(x) A(x) \phi_i(x) d^4x$$
 ...(82)

The field A(x) due to an electron at the site of the other electron is given by the Maxwell's equation:

$$\Box A_{\mu}(x) = -ie \, \overline{\phi}_{f}(x) \, \gamma_{\mu} \, \phi_{i}(x)$$

$$= -\frac{ie}{V} \cdot \sqrt{\left(\frac{m^{2}}{E_{1}E_{1}'}\right)} \cdot \overline{u}(p_{1}') \, \gamma_{\mu} \, u(p_{1}) \, e^{i(p_{1} - p_{1}') \cdot x}$$

$$\Rightarrow A(x) = \frac{ie}{V} \, \overline{u}(p_{1}') \, \gamma_{\mu} \, u(p_{1}) \, \frac{\exp \left(i(p_{1} - p_{1}') \cdot x\right)}{(p_{1} - p_{1}')^{2}} \cdot \sqrt{\left(\frac{m^{2}}{E_{1}E'}\right)}.$$

Hence the matrix element (82) becomes:

$$M^{(1)} = \frac{ie^{2}}{V^{2}} \frac{m^{2}}{\sqrt{(E_{1}E_{1}'E_{2}E_{2}')}} \cdot \bar{u}(\mathbf{p}_{1}') \, \gamma_{\mu} \, u \, (\mathbf{p}_{1})$$

$$\times \int d^{4}x \, e^{i \, (p_{1} - p_{1}' + p_{2} - p_{2}') \, x} \bar{u} \, (\mathbf{p}_{2}') \, \gamma_{\mu} \, u(\mathbf{p}_{2})$$

$$= \frac{ie^{2}}{V^{2}} (2\pi)^{4} \, \delta^{4} \, (p_{1} - p_{1}' + p_{2} - p_{2}') \, \frac{m^{2}}{\sqrt{(E_{1}E_{1}'E_{2}E_{2}')}}$$

$$\times \frac{[\bar{u} \, (\mathbf{p}_{1}') \, \gamma_{\mu} \, u \, (\mathbf{p}_{1})] \, [\bar{u} \, (\mathbf{p}_{2}') \, \gamma_{\mu} \, u \, (\mathbf{p}_{2})]}{(p_{1} - p_{1}')^{2}}$$

Similarly, for fig. 13 (b) we get the matrix element.

$$M^{(1)} = \frac{ie^{2}}{V^{2}} (2\pi)^{4} \delta^{4} (p_{1} \cdot p_{1}' + p_{2} + p_{2}') \frac{m^{2}}{\sqrt{(E_{1}E_{1}'E_{2}E_{2}')}} \times \frac{[\bar{u}(\mathbf{p}_{2}') \gamma_{\mu} u'\mathbf{p}_{1})] [\bar{u}(\mathbf{p}_{1}') \gamma_{\mu} u(\mathbf{p}_{2})]}{(p_{1} - p_{2}')^{2}}$$
Thus the section of the first circline int.

Thus the scattering amplitude for the electron-electron scattering, with spin labels suppressed is given by:

$$M^{(1)} = \frac{ie^{2}}{V^{2}} (2\pi)^{4} \delta^{4} (p_{1} + p_{2} - p_{1}' - p_{2}') \frac{m^{2}}{\sqrt{(E_{1}E_{1}'E_{2}E_{2}')}} \times \left[\frac{\bar{u}(\mathbf{p}_{1}') \gamma_{\mu} u(\mathbf{p}_{1}) \bar{u}(\mathbf{p}_{2}') \gamma_{\mu} u(\mathbf{p}_{2})}{(p_{1} - p_{1}')^{2}} - \frac{\bar{u}(\mathbf{p}_{2}') \gamma_{\mu} u(\mathbf{p}_{1}) \bar{u}(\mathbf{p}_{1}') \gamma_{\mu} u'(\mathbf{p}_{2})}{(p_{1} - p_{2}')^{2}} \right] ... (83)$$

The relative minus sign between the direct and the exchanged terms is due to the Fermi statistics, which requires the amplitude to be antisymmetric under interchange of the two final electrons. It is also antisymmetric under interchange of the two initial electrons as required by the statistics.

Thus the electron-electron scattering becomes more complicated due to addition of the exchange term compared to the electronproton scattering where we had only the direct term.

PROBLEMS

Problem 1. Average over the initial and sum over the final spin states of the electron and the proton to the Moller invariant cross-section (80).

Sol. We have

$$|\overline{M}|^2 = |\overline{u}(\mathbf{k}') \gamma_{\mu} u(\mathbf{k}) \frac{e^2}{q^2} \overline{u}(\mathbf{k}') \dot{\gamma}_{\nu} u(\mathbf{K})|^2$$

Averaging it over the initial and summing over the final states we obtain

we obtain
$$|\overline{M}|^{2} = \frac{1}{4} \sum_{k=1}^{\infty} \left[\overline{u(k')} \gamma_{\mu} u(k) \frac{e^{2}}{q^{2}} \overline{u(k')} \gamma_{\nu} u(k) \right] \times \left[\overline{u(k')} \gamma_{\mu} u(k) \frac{e^{2}}{q^{2}} \overline{u(k')} \gamma_{\nu} u(k) \right]^{\dagger}$$

$$= \frac{1}{4} \sum_{k=1}^{\infty} \left[\overline{u(k')} \gamma_{\mu} u(k) \frac{e^{2}}{q^{2}} \overline{u(k')} \gamma_{\nu} u(k) \right] \times \left[\overline{u(k)} \gamma_{\nu} u(k') \frac{e^{2}}{q^{2}} \overline{u(k)} \gamma_{\mu} u(k') \right]$$

$$= \frac{e^{4}}{4q^{4}} \sum_{k=1}^{\infty} \left\{ \overline{u(k')} \gamma_{\mu} u(k) \overline{u(k')} \gamma_{\mu} u(k) \overline{u(k)} \gamma_{\nu} u(k') \times \overline{u(k)} \gamma_{\mu} u(k') \right\}$$

$$= \frac{e^{4}}{4q^{4}} T_{r} \left[\gamma_{\mu} \frac{m - ik'}{2m} \gamma_{\nu} \frac{m - ik}{2m} \right] \times T_{r} \left[\gamma_{\mu} \frac{M - ik'}{2m} \gamma_{\nu} \frac{M - ik}{2m} \right] \dots (i)$$

Now,

$$T_{\mathbf{r}} \cdot \left[\gamma_{\mu} \frac{m - i k'}{2m} \gamma_{\nu} \frac{m - i k}{2m} \right] = \frac{1}{4m^{2}} T_{\mathbf{r}} \left[\gamma_{\mu} \left(m - i k' \right) \gamma_{\nu} \left(m - i k \right) \right]$$

$$= \frac{1}{4m^{2}} \left[T_{\mathbf{r}} \left(m^{2} \gamma_{\mu} \gamma_{\nu} \right) - T_{\mathbf{r}} \left(\gamma_{\mu} k' \gamma_{\nu} k \right) \right]$$
...(ii)

the trace of the product of an odd no. of y-matrices vanishes}

To evaluate the right hand side of (ii), we have

 $T_{\tau} (\gamma_{\mu} k' \gamma_{\nu} k) = k'_{\lambda} k \pi T_{\tau} (\gamma_{\mu} \gamma_{\lambda} \gamma_{\nu} \gamma_{\pi})$ $= k'_{\lambda} k_{\pi} \left(4\delta_{\mu\lambda} \delta_{\nu\pi} + 4\delta_{\mu\pi} \delta_{\lambda\nu} - 4\delta_{\mu\nu} \alpha_{\lambda\pi} \right)$

 $=4(k_{\mu}' k_{\nu} + k'_{\nu} k_{\mu} - k'_{\pi} k_{\pi} \delta_{\mu\nu})$

(ii) =
$$\frac{1}{m^2} \left[-k'_{\mu}k_{\nu} - k'_{\nu}k_{\mu} + \delta_{\mu\nu} (k' \cdot k + m^2) \right]$$

Similarly,

and

$$T_{r} \left[\gamma_{\mu} \frac{m - iK'}{2M} \gamma_{\nu} \frac{m - iK}{2M} \right] = \frac{1}{M^{2}} \left[-K'_{\mu} K_{\nu} - K_{\mu} K'_{\nu} + \delta_{\mu\nu} \times (K'.K + M^{2}) \right] ...(iii)$$

Multiplying (ii) and (iii), we get $|M|^2$ averaged over the final and summed over the initial spins. Using this value of $|\overline{M}|^2$ into (80), we the required result.

Problem. 2. Write down the matrix element for electron-positron scattering.

Sol. Feynman's graphs for positron-electron scattering is shown in the fig. 14 below.

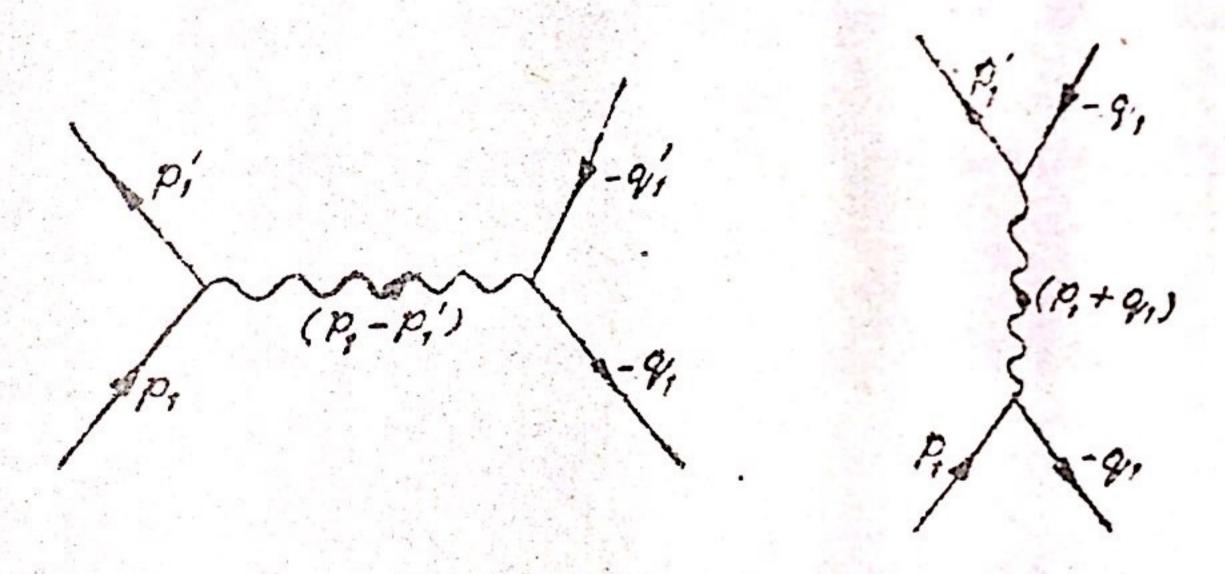


Fig. 14

We can consider the positron as an electron of negative energy moving backward in time. Hence the electron-positron scattering will be identical to the electron-electron scattering and the transition matrix element can be written analogously:

$$M^{(1)} = \frac{ie^{2}}{V^{2}} \cdot (2\pi)^{4} \delta^{4} \left(p'_{1} + q'_{1} - p_{1} - q_{1} \right) \cdot \frac{m^{2}}{\sqrt{(E_{p_{1}}E_{p_{1}}'E_{q_{1}}E_{q_{1}}')}} \times \left[\frac{u\left(\mathbf{p}_{1}'\right) \gamma_{\mu} u\left(\mathbf{p}_{1}\right) \overline{v\left(\mathbf{q}_{1}\right) \gamma_{\mu} v\left(\mathbf{q}_{1}'\right) \gamma_{\mu} v\left(\mathbf{q}_{1}'\right) \overline{v\left(\mathbf{q}_{1}\right) \gamma_{\mu} u\left(\mathbf{p}_{1}\right)}}{(p_{1} - p_{1}')^{2}} \frac{u\left(\mathbf{p}_{1}'\right) \gamma_{\mu} v\left(\mathbf{q}_{1}'\right) \gamma_{\mu} v\left(\mathbf{q}_{1}'\right) \overline{v\left(\mathbf{q}_{1}\right) \gamma_{\mu} u\left(\mathbf{p}_{1}\right)}}{(p_{1} + q_{1})^{2}} \right]$$

It is known as 'Bhabha amplitude'. The first term represents direct electron-positron scattering and the second term corresponds to the exchange scattering. The relative minus sign between the two terms comes due to the antisymmetry in the exchange of the electron with positive energy p_1 and the electron with negative energy $-q'_1$.

Problem 3. Show that the propagator $I(x_2-x_1)$ for a free K.G. particle satisfies equation (24).

[Hint: Do exactly in the same way as we did for a free Schroedinger particle].

We have seen that the transition from classical particle mechanics to the quantum machanics is doubly degenerate: We can develop the quantum theory from the classical particle mechanics, directly from the correspondence principle; i.e., by replacing the dynamical observables of the classical mechanics by their corresponding quantum mechanical operators. Operating these operators on the wavefunction, we can get all the desired information about the system. We can also develop a quantum theory in a straight forward manner, as in the case of Schroedinger's wave mechanics. Similarly, we can also develop a quantum theory for fields, either by using the correspondence principle or we can also formulate a quantum field theory directly from the quantum mechanics of the particles. Various paths to arrive at the 'Quantum field theory are depicted below:

However, we shall be developing a quantum theory of fields, directly from the classical theory of fields, using the correspondence principle. Thus, it will be useful to recall the elements of the classical theory of fields.

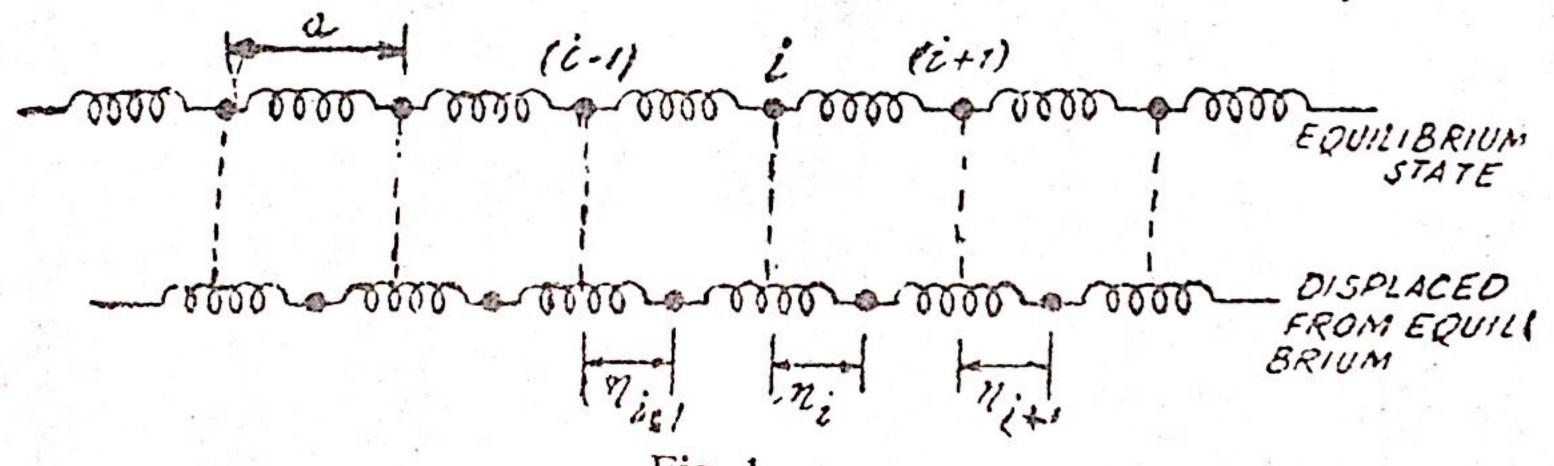
12.1. WHAT IS A FIELD

We are quite familiar with the word field in Physics. We know about the electric field, the magnetic field and the electromagnetic field etc. The electric field is characterized by specifying the value of the field strength E at all points of the space at a particular time. Similarly, the magnetic field is characterized by the field strength H and the electromagnetic field is characterized by the

vector potential A and the scalar potential \(\psi\). The values of E, H and ϕ for the electric, the magnetic and the electromagnetic fields; respectively, take on an infinite number of uncountable values. These can be considered as the degrees of freedom for these fields. The question immediately arises then, as to whether there are not other physical systems which have a non-denumerably infinite number of degrees of freedom. Indeed, there are a large number of such systems and these are known as fields. In general, the fields are continuous mechanical systems with a non denumerable infinite number of degrees of freedom. The degrees of freedom of a field is called the field functions and these assume the role of the generalized co-ordinates, qi, of a mechanical system with a finite number of degrees of freedom. As with any physical system, a field is the carrier of energy, momentum, angular momentum and other observable dynamical entities. The field propagates in accordance with the field equations of motion and thus carries with itself the dynamical observables.

12.2. TRANSITION FROM CLASSICAL MECHANICS: TO CLASSICAL FIELDS

The transition from classical mechanics to classical fields is equivalent to the transition from discontinuous to continuous variables. As an example, we consider to collection of N particles



connected with identical springs of force constant k and aligned in one dimension. By calling τ_l as the displacement of the ith particle from its equilibrium position, we can write the Lagrangian for the system of particles as

$$L = \frac{1}{2} \sum_{i=1}^{N} m \dot{\eta}_{i}^{2} - \frac{1}{2} k \sum_{i=1}^{N} (\eta_{i+1} - \eta_{i})^{2} \dots (1)$$

The first term on the right hand side gives the kinetic energy and the second term is the potential energy. 'm' is the mass of each particle. If 'a' is the equilibrium separation between the neighboring particles, we can write (1) as

$$L = \frac{1}{2} \sum_{i=1}^{N} a \cdot \frac{m}{a} \dot{\eta}_{i}^{2} - \frac{1}{2} k \sum_{i=1}^{N} a^{2} \left(\frac{\eta_{i+1} - \eta_{i}}{a} \right)^{2}$$

$$= \sum_{i=1}^{N} a L_{i};$$

$$= \sum_{i=1}^{N} a L_{i};$$

$$(2)$$

where,

$$L_{i} = \frac{1}{2} \left[\frac{m}{a} \dot{\eta}_{i}^{2} - ka \left(\frac{\eta_{i+1} - \eta_{i}}{a} \right)^{2} \right]$$

$$\dots (3)$$

is the Lagrangian per unit length; i.e., the linear Lagrangian density.

Now, we can transit to a continuous system from this discrete mechanical system by making the number of degrees of freedom as infinite in such a way that the separation distance becomes infinitesimal:

$$N \to \infty$$
; $a \to dx$; $\frac{m}{a} \to \mu$, linear mass density;

$$\frac{\eta_{i+1} - \eta_i}{a} \rightarrow \frac{d \eta_i(x)}{dx}$$
; $ka \rightarrow Y$, Young's modulus.

We thus have

$$L=\int L dx,$$
 ... (4)

where

$$L = \frac{1}{2} \left[\mu \dot{\eta}^2 - Y \left(\frac{d\eta}{dx} \right)^2 \right]. \tag{5}$$

We note that η itself has become a function of the continuous parameter 'x'.

From the above mechanical example, we can label the field functions instantaneously. The Lagrangian in classical mechanics is written as $L(q_i(t), \dot{q}_i(t))$. To describe the infinite number of degrees of freedom of the field, we replace the generalized coordinates $q_i(t)$ by a continuous function $\psi(x, t)$, of the variables x

†If the force F exerted on a rod leads to an extension l per unit length, then F = Yl, where Y is the Young's modulus. Now the force required to stretch the spring of original length a is given by

$$F=k (\eta_{i+1}-\eta_i)=ka\frac{\eta_{i+1}-\eta_i}{a}=kal.$$

Therefore, taking analogy from the continuous rod, here, for the discrete system, ka corresponds to the Young's modulus.

and t for a one dimensional field. The analogy becomes more apparent if we think $\psi(x, t)$ as $\psi_x(t)$, where the discrete labelling 'i' for the particles has been replaced by a continuously varying parameter 'x' in case of the fields. Thus

$$\frac{q_i(t) \to \psi(x, t)}{\dot{q}_i(t) \to \frac{d\psi(x, t)}{dt}}, \frac{d\psi(x, t)}{\dot{d}x} \right\} \dots (6)$$

Since in actual practice, the fields are three dimensional systems, we write the field functions as $\psi(x, t)$, where x is the position vector with the components x, y and z. The analogy (6) now becomes

$$q_i(t) \rightarrow \psi(\mathbf{x}, t)$$
 $\dot{q}_i(t) \rightarrow \frac{\partial \psi}{\partial x_{\mu}}$:

where x_{μ} is the space-time four-vector with the components $x_1 = x$, $x_2 = y$, $x_3 = z$ and $x_4 = ict.\dagger$

Thus the Lagrangian for the fields can be written in analogy with $L(q_i, \dot{q}_i)$ as

$$L\left(\psi,\frac{\partial\psi}{\partial x_{\mu}}\right). \qquad ...(7)$$

Defining a Lagrangian density $\mathbf{L}\left(\psi, \frac{\partial \psi}{\partial \psi_{\mu}}\right)$ for the field we can write

$$L\left(\psi,\frac{\partial\psi}{\partial x_{\mu}}\right) = \int L\left(\psi,\frac{\partial\psi}{\partial x_{\mu}}\right) d^3x, \qquad \dots (8)$$

where $d^3x = dx_1 dx_2 dx_3$.

The action for the field can be defined, in an analogous manner to that for the classical particle mechanics, as

$$I = \int_{t_1}^{t_2} L \ dt = \iint \mathbf{L} \left(\psi, \frac{\partial \psi}{\partial x_{\nu}} \right) d^3x \ dt. \tag{9}$$

12.3. EULER LAGRANGE'S EQUATIONS OF MOTION:

We can derive the Lagrange's equations of motion for the fields from the Hamilton's variational principle, according to which the variation of (9) must be zero, i.e.,

[†]The sign convention will be used according to which the Greek indices μ , ν , λ etc. will be understood to take values from 1 to 4 and the italic indices i, j, k etc. will be understood to take the values from 1 to 3. There will be understood summation over the repeated indices μ , ν , λ etc. from 1 to 4 and the repeated indices i, j, k etc. from 1 to 3.

or
$$\int \int \partial \int \partial u du = 0$$

$$\int \int \int \int \partial u du = 0$$

$$\int \int \int \partial u du = 0$$

$$\int \int \int \partial u du = 0$$

$$\int \partial$$

We can find the variation $\delta\left(\frac{\partial\psi}{\partial x_{\mu}}\right)$ in two ways:

First, suppose ψ varies by $\delta \psi$ and becomes $\psi' = \psi + \delta \psi$.

$$\therefore \frac{\partial \psi'}{\partial x_{\mu}} = \frac{\partial \psi}{\partial x_{\mu}} + \frac{\partial (\delta \psi)}{\partial x_{\mu}}.$$
 (12)

Secondly, suppose $\frac{\partial \psi}{\partial x_{\mu}}$ varies by $\delta\left(\frac{\partial \psi}{\partial x_{\mu}}\right)$ and becomes

$$\frac{\partial \psi'}{\partial x_{\mu}} = \frac{\partial \psi}{\partial x_{\mu}} + \delta \left(\frac{\partial \psi}{\partial x_{\mu}} \right). \tag{13}$$

Comparing (12) and (13), we have

$$\delta \left(\frac{\partial \psi}{\partial x_{\mu}} \right) = \frac{\partial \left(\delta \psi \right)}{\partial x_{\mu}}.$$

Using it and introducing the notation $\frac{\partial}{\partial x_{\mu}} \equiv \partial_{\mu}$, we can write (11) as

$$\iint d^3x \ dt \left[\frac{\partial L}{\partial \psi} \delta \psi + \frac{\partial L}{\partial (\partial_{\mu} \psi)} \partial_{\mu} (\delta \psi) \right] = 0. \tag{14}$$

The second term in the above equation can be evaluated by integrating by parts

$$\iint d^3x \ dt \ \frac{\partial L}{\partial (\partial_{\mu}\psi)} \partial_{\mu} (\delta\psi) = \int_{\Sigma} d\sigma \frac{\partial L}{\partial (\partial_{\mu}\psi)} \delta\psi \hat{n} (\mathbf{r})$$
$$-\iint_{\Omega} d^3x \ dt \ \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu}\psi)} \right) \delta\psi. \qquad \dots (15)$$

Here Σ denotes the surface of the four dimensional volume Ω and $\hat{n}(\mathbf{x})$ is the ourward drawn normal to this surface at the point \mathbf{x} .

The surface integral in (15) vanishes because the variation $\delta\psi$ is zero at the ends t_1 and t_2 . Therefore

$$\iint d^3x \ dt \left[\frac{\partial L}{\partial \psi} - \frac{\partial}{\partial x_F} \left(\frac{\partial L}{\partial (\partial_\mu \psi)} \right) \right] \delta \psi = 0. \tag{16}$$

Since $\delta\psi$ is an arbitrary variation at each point in space and hence it cannot be zero in general. Thus we must have

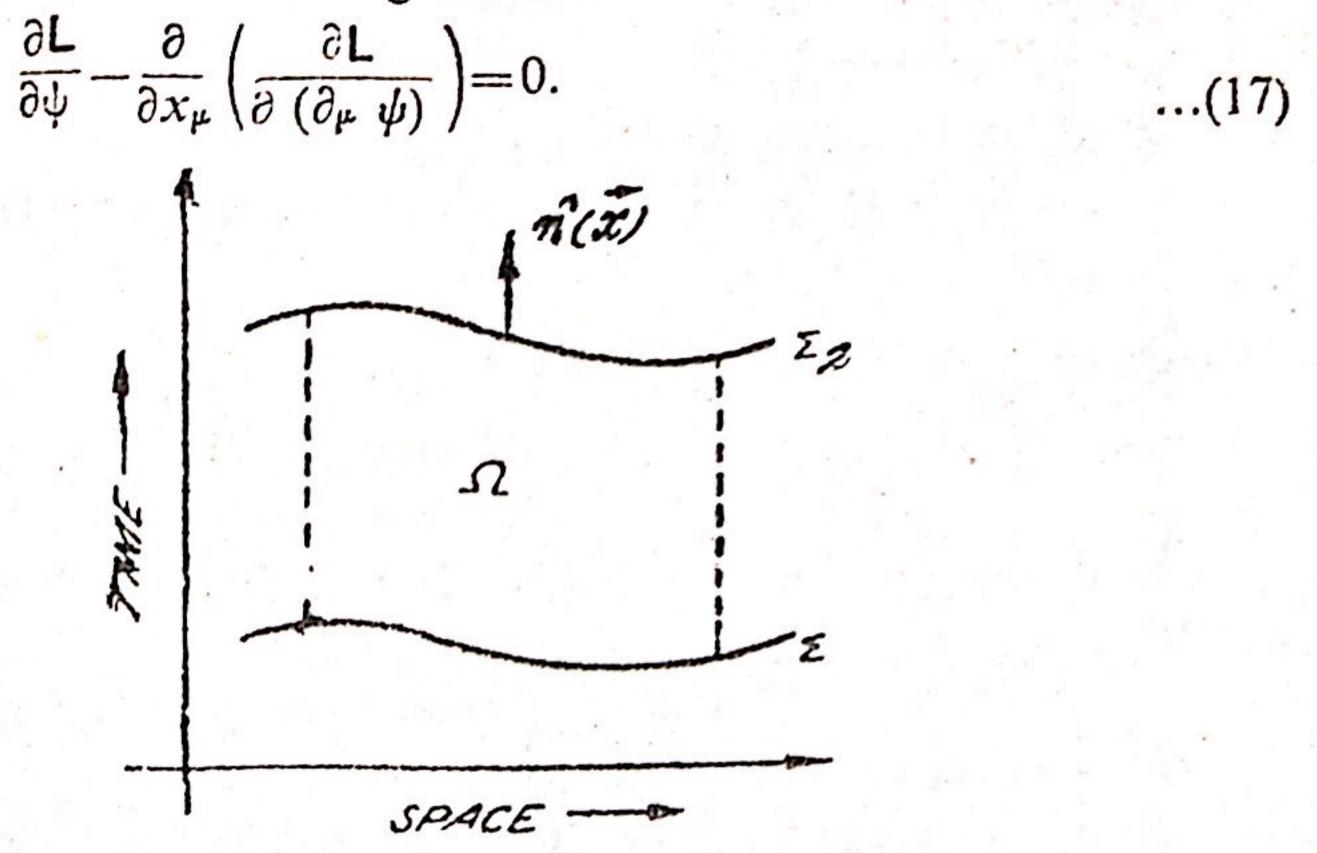


Fig. 2.

This is the Euler Lagrange's equation for the field with field function ψ and Lagrangian density L. If the field function has many components*, these can be specified by a suffix with it as

$$\psi_{\alpha} (\alpha = 1, 2, ..., N),$$

i.e. here ψ has N components. Each component of ψ satisfies a Euler Lagrange's equation of the form (17), i.e.

$$\frac{\partial L}{\partial \psi_{\alpha}} - \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \psi_{\alpha})} \right) = 0 \; ; \; \alpha = 1, 2, ..., N$$
 ...(18)

To write (17) in a more analogous form to the classical lagrange's equation, we transform it in terms of the total Lagrang-

ian L. We define the functional derivatives $\frac{\partial L}{\partial \psi}$ and $\frac{\partial L}{\partial \psi}$, as

$$\frac{\partial L}{\partial \psi} \text{ and } \frac{\partial L}{\partial \psi} = \lim_{d^3 x \to 0} \frac{\delta L}{\delta \psi d^3 x} \text{ and } \lim_{d^3 x \to 0} \frac{\delta L}{\delta \psi d^3 x} \qquad \dots (19)$$
Now,

$$L = \int d^3x \, \mathbf{L} \left(\psi, \frac{\partial \psi}{\partial x_{\mu}} \right)$$

$$\therefore \quad \delta L = \int d^3x \, \left[\frac{\partial \mathbf{L}}{\partial \psi} \, \delta \psi + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \psi)} \partial_{\mu} (\delta \psi) \right]$$

^{*}The electromagnetic field is an example of fields with more than one component It is described by four potential $A_{\mu} = A_1$, A_2 , A_3 , $i\phi$, (N=4), where A_1 , A_2 , A_3 are the three comonents of the vector potential A and ϕ is the scalar potential.

$$= \int d^3x \left[\frac{\partial \mathbf{L}}{\partial \psi} \delta \psi + \frac{\partial \mathbf{L}}{\partial (\partial_i \psi)} \partial_i (\delta \psi) + \frac{\partial \mathbf{L}}{\partial (\partial_4 \psi)} \partial_4 (\delta \psi) \right]$$

$$= \int d^3x \left[\frac{\partial \mathbf{L}}{\partial \psi} \delta \psi + \frac{\partial \mathbf{L}}{\partial (\partial_i \psi)} \partial_i (\delta \psi) + \frac{\partial \mathbf{L}}{\partial \psi} \delta \psi \right] \{ \because x_4 \equiv ict \}$$

In the above eqn. summation over the dummy index 'i' is to be understood from i=1 to 3.

Integ ating the middle term on the right hand side of the above equation by parts and noting that the surface term will vanish over the infinite surface of integration, we obtain,

$$\delta L = \int d^3x \left[\frac{\partial L}{\partial \psi} \delta \psi - \frac{\partial}{\partial x_i} \left(\frac{\partial L}{\partial (\partial_i \psi)} \right) \delta \psi + \frac{\partial L}{\partial \psi} \delta \psi \right],$$

where the variation in L is now produced by independent variation in ψ and $\dot{\psi}$. Therefore,

$$\frac{\partial L}{\partial \psi} = \frac{\partial L}{\partial \psi} - \frac{\partial}{\partial x_{i}} \left(\frac{\partial L}{\partial (\partial_{i} \psi)} \right) \dots (20)$$

$$\frac{\partial L}{\partial \psi} = \frac{\partial L}{\partial \psi} = \frac{\partial L}{\partial \psi}$$

Using (20) in (17) we can write:

$$\frac{\partial L}{\partial \psi} - \frac{\partial}{\partial x_{i}} \left(\frac{\partial L}{\partial (\partial_{i} \psi)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial (\dot{\psi})} \right) = 0$$

$$\frac{\partial L}{\partial \psi} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{\psi}} \right) = 0$$

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{\psi}} \right) = \frac{\partial L}{\partial \psi} \qquad ...(21)$$

or

or

This equation resembles the Lagranges eqn. for a system of particles

$$\frac{d}{dt} \left(\frac{\partial \mathbf{L}}{\partial \dot{q}_i} \right) = \frac{\partial L}{\partial q_i} \; ; \; i = 1, 2, 3, ..., N. \qquad ...(22)$$

12.4. CANONICAL CO-ORDINATES FOR THE FIELDS:

In classical mechanics we define the canonical momentum from the Lagrangian $L(q_i.\dot{q_i})$ as:

$$p_{i} = \frac{\partial L}{\partial q_{i}}$$

Similary, in classical field theory we can define the canonical conjugate momentum density π_{μ} as:

$$\pi_{\mu} = \frac{\partial \mathbf{L}}{\partial(\partial_{\mu}\psi)} \qquad (23a)$$

For an N-component field, the components of the mementum density are given by:

$$\pi_{\mu\alpha} = \frac{\partial \mathbf{L}}{\partial (\partial_{\mu}\psi_{\alpha})}$$
; $\alpha = 1, 2, ..., N$(23b)

Since the Hamiltonian should represent the total energy, in real practice, it is useful to define the momentum density, only by the time derivative as

$$\pi = \frac{\partial \mathbf{L}}{\partial \dot{\psi}},$$
 ...(24-a)

and

$$\pi_{\alpha} = \frac{\partial \mathbf{L}}{\partial \dot{\psi}_{\alpha}}$$
; $\alpha = 1, 2, \dots, N$(24-b)

In analogy with the Hamiltonian ' $H = \sum_{i} p_{i}q_{i} - L$ in classical mechanics the Hamiltonian density for the classical fields can be written as:

 $H = \pi \dot{\psi} - L$, for a single component field

and

$$H = \sum_{\alpha=1}^{N} \pi_{\alpha} \dot{\varphi}_{\alpha} - L$$
, for multi-component field. ...(25-b)

The total Hamiltonian for the field is given by:

$$H = \int H d^3x \qquad ...(26)$$

Also, the Hamilton's eqns. of motion for the canonical variables ψ_{α} and τ_{α} can be written as:

$$\dot{\pi}_{\alpha}(x, t) = -\frac{\partial H}{\partial \dot{\sigma}_{\alpha}}; \qquad ...(27-a)$$

$$\dot{\psi}_{\alpha}(x, t) = \frac{\partial H}{\partial \pi_{\alpha}}; \qquad ...(27-b)$$

$$\alpha = 1, 2, ..., N.$$

12.5. REAL SCALAR FIELD:

As a particular example, we consider the real scalar field in this section. In the succeeding sections we shall discuss some more examples of the fields.

The scalar field is one which remains unchanged under Lorentz transformation: i.e., the field function $\phi(x, t)$ transforms like

$$\phi'(\mathbf{x}',t') = \phi(\mathbf{x},t)$$

under a Lorentz transformation. If the field functions $\phi(x, t)$ is real we have a real scalar field.

In the preceding sections we have used the covariant notations. The Lagrangian, the Hamiltonian and the Lagrange's and the Hamilton's equations of motion are all written in covariant notations. The field function ϕ is also considered as a function of the covariant variable x_{μ} . We did it with the presumption that the field equations, being the laws of Nature, should be covariant under a proper Lorentz transformation. However, the covariance is not sufficient to completely determine the form of the possible field equations. We also make the following simplifying assumptions in order to eliminate the complications:

- (a) We shall deal with local fields only; i.e., the state of the field, and the interaction of fields at a given space time point, will be completely known from field functions $\varphi(x_{\mu})$ and their derivatives evaluated at the particular point, and won't depend on neighbourhood of the point.
- (b) We assume that the interaction-free-field eqns. are linear in the field functions and their derivatives. The non-linear terms are tantamount to an interaction. Therefore, requiring linearity is equivalent to sorbidding a self-interaction of a specified isolated field.
- We assume that the field equations are of the lowest possible order; i.e., they are at most second order differential equations. The higher order terms in the field equations have essentially the same effect as non-linear terms.

We shall now develop the equation for the scalar field under the above restrictions. Due to the linearity requirement for the field equations, L must quadratic function of p and $\frac{\partial p}{\partial x}$. Therefore, φ^2 and $(\partial_{\mu}\varphi)$ $(\partial_{\mu}\varphi)$ will do for L. We cannot take φ . $(\partial_{\mu}\psi)$, because it is not Lorentz covariant. Hence the Lagrangian density for the scalar field can be written as

$$L = A\varphi^2 + B(\partial_{\mu}\varphi)^2;$$

where A and B are certain constants.

...(28)

Separating the time part of $(\partial_{\mu}\varphi)^2$ we write,

 $L = Ap^2 + B \left[(\partial_i \varphi)^2 - \varphi^2 \right]$

We have taken c=1 here, and in what follows we shall be using the natural units.

From (29) we have the momentum density

$$\pi = \frac{\dot{c}\mathbf{L}}{\dot{c}\dot{\varphi}} = -2B\dot{\varphi} \Rightarrow \dot{\varphi} = -\frac{\pi}{2B} \qquad ...(30)$$

Hence the Hamiltonian density can be written as

$$H = \pi \dot{\varphi} - L = -\frac{\pi^2}{2B} - A\varphi^2 - B(\partial_i \varphi)^2 + \frac{\pi^2}{4B}. \qquad ...(31)$$

As H gives the total energy density of the field, it should be positive definite. Thus A and B should both be real and negative.

From (28) we can write the Euler Lagrange's eqn. of motion for the real scalar field,

$$\frac{\partial \mathbf{L}}{\partial \varphi} = \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial \mathbf{L}}{\partial \partial_{\mu} \varphi} \right)$$

$$\therefore 2A\varphi = 2B \partial_{\mu}^{2} \varphi = 2B \square \varphi; \quad \square = \partial_{\mu}^{2} = \nabla^{2} - \frac{1}{c^{2}} \frac{\partial^{2}}{\partial t^{2}}$$

$$\square \varphi - \left(\frac{A}{B} \right) \varphi = 0 \qquad ...(32)$$

This equation is of the form of the Klein-Gordon equation, $\Box \varphi - \frac{m^2c^2}{\ln^2}\varphi = 0.$ Let us now investigate the significance of the constant $\left(\frac{A}{B}\right)$ here. It should be real and positive because both of A and B are real and negative. Also, from the principle of homogeneity for dimensions, it should have the dimensions of the inverse length square. At quantum level, comparing (32) with the Klein-Gordon equation, we have

$$\left(\frac{A}{B}\right) = \frac{m^2c^2}{\hbar^2} = \frac{1}{(\text{Compton wave length})^2}$$
:

i.e., the dimensions of $\left(\frac{A}{B}\right)$ is that of inverse length square.

Hence, in terms of the natural units, $\left(\frac{A}{B}\right)$ can be recognized as the square of the mass at quantum level. With this speculation we write $\left(\frac{A}{B}\right) = m^2$ here, so that m can be recognized as the mass when we shall study the quantization of this field.

Now defining a new field functions $\Phi = \sqrt{(-2B)} \varphi$, † we can write the Lagrangian for the real scalar field as:

$$L = -\frac{1}{2} (\partial_{\mu} \Phi)^{2} - \frac{1}{2} \left(\frac{A}{B}\right) \Phi^{2}$$

$$L = -\frac{1}{2} (\partial_{\mu} \Phi)^{2} - \frac{1}{2} m^{2} \Phi^{2} \qquad ...(33)$$

or

or

For a multi-component scalar field we write

$$L = -\frac{1}{2}m^2 \Phi_{\alpha}^2 - \frac{1}{2} (\hat{\sigma}_{\mu} \Phi_{\alpha})^2, \ \alpha = 1, 2, ...N. \qquad ...(34)$$

⁺Multiplying the field functions by some constant is equivalent to multiplying the Lagrangian density by that constant. As the field equations of motion do not change by multiplying the Lagrangian by a constant, defining the field functions as $\Phi = \sqrt{(-2B)} \varphi$ makes ro change in the formalism.

Separating the time part, Lagrangian density (33) can be written as:

$$L = \frac{1}{2} \dot{\Phi}^2 - \frac{1}{2} (\nabla \Phi)^2 - \frac{1}{2} m^2 \Phi^2 \qquad ...(35)$$

Using this, Hamiltonian density is given as:

$$H = \pi \dot{\Phi} - L = \pi \dot{\Phi} - \frac{1}{2} \dot{\Phi}^2 + \frac{1}{2} (\nabla \Phi)^2 + \frac{1}{2} m^2 \dot{\Phi}^2 \qquad ...(36)$$

From (35), we have

$$\pi = \frac{\partial L}{\partial \dot{\Phi}} = \dot{\Phi}$$

Using it into (36), we get

$$\begin{aligned}
&H = \pi \cdot \pi - \frac{1}{2}\pi^2 + \frac{1}{2} (\nabla \Phi)^2 + \frac{1}{2}m^2 \Phi^2 \\
&= \frac{1}{2} \left[\pi^2 + (\nabla \Phi)^2 + m^2 \Phi^2 \right] & \dots (37)
\end{aligned}$$

12.6. COMPLEX SCALAR FIELD:

If the field functions, ϕ , of a scalar field are complex, then we have a complex scalar field. We can write ϕ by splitting it into the real and the imaginary parts:

$$\phi = \frac{\phi_1 + i\phi_2}{\sqrt{(2)}};$$

$$\phi^* = \frac{\phi_1 - i\phi_2}{\sqrt{(2)}}, \qquad ...(38)$$

and

where ϕ_1 and ϕ_2 are real scalar fields.

The free field Lagrangian density for the complex field can be written, not only as a function of ϕ and ϕ^* , but also as a function of ϕ_1 and ϕ_2 ; i.e., we may vary $L(\phi, \partial_\mu \phi, \phi^*, \partial_\mu \phi^*)$ independently with respect to ϕ and ϕ^* ; which is equivalent to varying $L(\phi_1, \partial_\mu \phi_1, \phi_2, \partial_\mu \phi_2)$ independently with respect to ϕ_1 and ϕ_2 .

From (38) we have,

$$\phi_{1} = \frac{\phi + \phi^{*}}{\sqrt{(2)}};$$

$$\phi_{2} = \frac{\phi - \phi^{*}}{\sqrt{(2)}i};$$

and

As ϕ_1 and ϕ_2 are real, therefore, using the expression (33) for the Lagrangian density of a real scalar field, the Lagrangian density for the complex scalar field can be written in terms of ϕ and ϕ^* as

$$L = -\frac{1}{2}m_{1}^{2} \left(\frac{\phi + \phi^{*}}{\sqrt{2}}\right)^{2} - \frac{1}{2}m_{2}^{2} \left(\frac{\phi - \phi^{*}}{\sqrt{2}.i}\right)^{2}$$

$$-\frac{1}{2} \left[\partial_{\mu} \left(\frac{\phi + \phi^{*}}{\sqrt{2}}\right)\right]^{2} - \frac{1}{2} \left[\partial_{\mu} \left(\frac{\phi - \phi^{*}}{\sqrt{2}.i}\right)\right]^{2};$$

where m_1 and m_2 are the masses of the real fields ϕ_1 and ϕ_2 ; respectively. If $m_1 \neq m_2$, then we cannot give any physical interpretation to the complex scalar field. Hence we take $m_1 = m_2 = m$ (say) and write

$$L = -m^2 \phi^* \phi - (\partial_{\mu} \phi^*) (\partial_{\mu} \phi) \qquad ... (39)$$

for the Lagrangian density of the complex scalar field in terms of ϕ and ϕ^* .

The Euler Lagrange's equations can be obtained by treating ϕ and ϕ^* as two independent fields:

$$\frac{\partial L}{\partial \phi} = \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \phi)} \right) \Rightarrow \Box \phi^* - m^2 \phi^* = 0,$$

$$\frac{\partial L}{\partial \phi^*} = \frac{\partial}{\partial x_{\mu}} \left[\frac{\partial L}{\partial (\partial_{\mu} \phi^*)} \right] \Rightarrow \Box \phi - m^2 \phi = 0.$$
...(40)

and

The canonically conjugate momenta are given by

$$\pi = \frac{\partial L}{\partial \dot{\phi}} = \dot{\phi}^*$$
; $\pi^* = \frac{\partial L}{\partial \dot{\phi}^*} = \dot{\phi}$

and hence the Hamiltonian density can be written as:

$$\mathbf{H} = \pi \dot{\phi} + \pi^* \dot{\phi}^* - \mathbf{L}
= (\pi \pi^* + \pi^* \pi) - (\pi \pi^* - \nabla \phi^* \cdot \nabla \phi - m^2 \phi^* \phi)
= \pi^* \pi + (\nabla \phi^*) \cdot (\nabla \phi) + m^2 \phi^* \phi \qquad ...(41)$$

Clearly, it is positive definite.

For a multicomponent complex field, the Lagrangian density, the equations of motion and the Hamiltonian density can be written as

$$L = -m^2 \phi^*_{\alpha} \phi_{\alpha} - \partial_{\mu} \phi^*_{\alpha} \cdot \partial_{\mu} \phi_{\alpha}, \qquad \dots (39')$$

$$\Box \phi^*_{\alpha} - m^2 \phi_{\alpha}^* = 0,$$

$$\Box \dot{\phi}_{\alpha} - m^2 \phi_{\alpha} = 0, \qquad \dots (40')$$

and

$$H = \pi^*_{\alpha} \pi_{\alpha} + (\nabla \phi_{\alpha}^*) \cdot (\nabla \phi_{\alpha}) + m^2 \phi^*_{\alpha} \phi_{\alpha} \qquad ...(41')$$

What is the physical significance of a complex field? To see it, we observe that the Lagrangian density (39) is invariant under the transformation

and
$$\phi \to \phi \ e^{i\epsilon} \approx \phi \ (1+i\epsilon),$$

 $\phi^* \to \phi^* \ e^{-i\epsilon} \approx \phi^* \ (1-i\epsilon).$...(42)

where ϵ is an infinitesimal real constant. This is called, after W. Pauli, the gauge transformation of the first kind.

From (42), we have

$$\delta \phi = i\epsilon \phi, \ \delta \phi^* = -i\epsilon \phi^* \qquad ...(43)$$

for the variations in ϕ and ϕ^* .

The change in L (ϕ , $\partial_{\mu}\phi$, ϕ^* , $\partial_{\mu}\phi^*$) due to variations of $\delta\phi$ and $\delta\phi^*$ is given by

$$\delta \mathbf{L} = \frac{\partial \mathbf{L}}{\partial \phi} \delta \phi + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi)} \delta (\partial_{\mu} \phi) + \frac{\partial \mathbf{L}}{\partial \phi^{*}} \delta \phi^{*} + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi^{*})} \delta (\partial_{\mu} \phi^{*})$$

$$= \frac{\partial \mathbf{L}}{\partial \phi} \delta \phi + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi)} \partial_{\mu} (\delta \phi) + \frac{\partial \mathbf{L}}{\partial \phi^{*}} \delta \phi^{*} + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi^{*})} \partial_{\mu} (\delta \phi^{*})$$

$$\{ :: \delta (\partial_{\mu} \phi) = \partial_{\mu} (\delta \phi) \}$$

$$= \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi)} \right) \delta \phi + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi)} \partial_{\mu} (\delta \phi) + \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi^{*})} \right) \delta \phi^{*}$$

$$+ \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi^{*})} \partial_{\mu} (\delta \phi^{*}) \qquad \{ \text{Using (40)} \}$$

$$= \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi)} \delta \phi + \frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \phi^{*})} \delta \phi^{*} \right)$$

Since the Lagrangian density is known to be unchanged from our earlier argument; δL must be zero. Thus we have the important result

or
$$\frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \phi)} \delta \phi + \frac{\partial L}{\partial (\partial_{\mu} \phi^{*})} \delta \phi^{*} \right) = 0$$
or
$$i\epsilon \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \phi)} \phi - \frac{\partial L}{\partial (\partial_{\mu} \phi^{*})} \phi^{*} \right) = 0$$
or
$$\frac{\partial j_{\mu}}{\partial x_{\mu}} = 0$$
where,
$$\frac{\partial j_{\mu}}{\partial x_{\mu}} = 0$$
...(44)

$$j_{\mu} = i\epsilon \left(\frac{\partial L}{\partial (\partial_{\mu} \phi)} \phi - \frac{\partial L}{\partial (\partial_{\mu} \phi^{*})} \phi^{*} \right)$$

$$= i\epsilon \left[(\partial_{\mu} \phi) \phi^{*} - (\partial_{\mu} \phi^{*}) \phi \right] \equiv i\epsilon \left(\phi^{*} \partial_{\mu} \phi \right) \dots (45)$$

can be interpreted as the conserved four-vector current associated with a complex scalar field ϕ . Eqn. (44) is the continuity equation satisfied by the four-vector charge-current density j_{μ} . We have

$$j_{k} = i\epsilon \left(\frac{\partial \phi}{\partial x_{k}} \phi^{*} - \frac{\partial \phi^{*}}{\partial x_{k}} \phi \right) \qquad ...(46a)$$

$$j_{4} = i\epsilon \left(\dot{\phi} \phi^{*} - \dot{\phi}^{*} \phi \right) \qquad ...(46b)$$

Eqns. (46 a) and (46 b) express charge and current density for the complex field.

Equation (44) defines a constant of motion $\int j_4(x) d^3x$. For the gauge transformation of first kind, this constant corresponds to the total charge Q.

Thus we see that a complex field describes the charged system. Therefore, it is also called as a charged scalar field. A real field cannot describe the charged system. Because, $\phi^* = \phi$ for the real field and hence, we get

$$j_{\mu} \equiv 0$$

Thus a real scalar field describes only the neutral systems. Therefore, it is also called as the neutral scalar field.

12.7. SCHROEDINGER'S FIELD:

The Schroedinger's wave mechanical equation of motion is given by

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{r}, t) \cdot \psi \qquad ...(47)$$

The field described by ψ and satisfying eqn. (47) is known as the Schroedinger's field.

The free field Lagrangian density, from which the field equation (47) may be derived, is given by

$$L = -i\hbar \psi^* \dot{\psi} - \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi - V(\mathbf{r}, t) \psi^* \psi \qquad ...(48)$$

From (48), we have

$$\frac{\partial L}{\partial \psi} = -V\psi^* ; \frac{\partial L}{\partial (\partial_k \psi)} = \frac{\partial L}{\partial (\nabla \psi)} = -\frac{\hbar^2}{2m} \nabla \psi^* ; \frac{\partial L}{\partial \psi} = i\hbar \psi^*$$

Hence the Euler Lagrange's equation is found to be

$$i\hbar \dot{\psi}^* - \frac{\hbar^2}{2m} \nabla^2 \psi^* = -V\psi^*$$

or

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^*, \qquad ...(49)$$

which is the complex cojugate of Schroedinger eqn. (47). Similarly, variation of ψ^* gives the eqn. (47).

The "canonical momentum density" π conjugate to ψ is given by

$$\pi = \frac{\partial L}{\partial \dot{\psi}} i\hbar \psi^*$$

And, the Hamiltonian density is given from eqn. (25) as:

$$\mathbf{H} = \pi \dot{\psi} - \mathbf{L} = i\hbar \ \psi^* \dot{\psi} - i\hbar \psi^* \dot{\psi} + \frac{\hbar^2}{2m} \ \nabla \psi^* \cdot \nabla \psi + V \psi^* \psi$$

$$= \frac{\hbar^2}{2m} \ \nabla \psi^* \cdot \nabla \psi + V \psi^* \psi$$

$$= -\frac{i\hbar}{2m} \nabla \pi \cdot \nabla \psi - \frac{i}{\hbar} V \pi \psi$$
...(50)

Hamilton's eqns. of motion (27) are:

$$\dot{\psi} = -\frac{i}{\hbar} V \psi + \frac{i\hbar}{2m} \nabla^2 \psi; \ \dot{\pi} = \frac{i}{\hbar} V \pi - \frac{i\hbar}{2m} \nabla^2 \pi \qquad ...(51)$$

12.8. DIRAC'S FIELD:

The Dirac field is described by the spinor wavefunctions ψ and $\overline{\psi}$ satisfying the field equations:

$$(\gamma_{\mu} \overrightarrow{\partial}_{\mu} + m) \psi = 0,$$

and $\overline{\psi} (-\gamma_{\mu} \overrightarrow{\partial}_{\mu} + m) = 0$...(52)

The free field Lagrangian density, from which the field equations may be derived, is given by:

$$\mathbf{L} = -\overline{\psi} \left(\gamma_{\mu} \stackrel{\rightarrow}{\partial_{\mu}} + m \right) \psi$$

$$= -\overline{\psi}_{\alpha} \left\{ (\gamma_{\mu})_{\alpha\beta} \stackrel{\rightarrow}{\partial_{\mu}} + m \delta_{\alpha\beta} \right\} \psi_{\beta}, \qquad \dots (53)$$

which is a Lorentz invariant scalar density. In the Lagrangian formulation each of the four components of ψ and $\overline{\psi}$ is to be regarded as an independent field variable. From (53) we have

 $\frac{\partial \mathbf{L}}{\partial \bar{\psi}_{\alpha}} = -(\gamma_{\mu} \partial_{\mu} \psi)_{\alpha} - m\psi_{\alpha}$ $\frac{\partial \mathbf{L}}{\partial (\partial_{\mu} \bar{\psi}_{\alpha})} = 0$

and

Hence the Euler Lagrange's equation is given by

$$(\gamma_{\mu} \overrightarrow{\partial}_{\mu} + m) \psi = 0 \qquad ...(54a)$$

Similarly, variation of \(\psi \) gives:

$$\frac{\partial L}{\partial \psi_{\beta}} = -\bar{\psi}_{\beta} m$$
, and $\frac{\partial L}{\partial (\partial_{\mu}\psi_{\beta})} = -(\bar{\psi}\gamma_{\mu})_{\beta}$

Therefore, the Euler Lagrange's eqn. is:

 $-\partial_{\mu}(\bar{\psi}\gamma_{\mu})_{\beta} = -m\bar{\psi}_{\beta}$ $\bar{\psi}(-\gamma_{\mu} \partial_{\mu} + m) = 0 \qquad ...(54b)$

or

Eqns. (54.a) and (54b) are exactly the Dirac eqn. and its adjoint; respectively. Thus the field eqns. can be derived from the Lagrangian density (53).

The "canonical momentum density" π conjugate to ψ is given by

$$\pi_{\beta} = \frac{\partial L}{\partial \dot{\psi}_{\beta}} = i \overline{\psi}_{\alpha} (\gamma_{4})_{\alpha\beta} = t \psi_{\beta}^{\dagger}$$

The canonical momentum conjugate to $\overline{\psi}$ vanishes. The Hamiltoian density is now given by:

$$H = \pi_{\beta}\dot{\psi}_{\beta} - \mathbf{L}$$

$$= \left(i\dot{\psi}^{\dagger}\dot{\psi} - i\overline{\psi}\,\gamma_{4}\dot{\psi} + \overline{\psi}\,\gamma_{k}\frac{\partial\psi}{\partial x_{k}} + m\overline{\psi}\psi\right)$$

$$= \psi^{\dagger}(-ix.\nabla + m\beta)\,\psi \qquad ...(55)$$

Thus the total Hamiltonian of the free Dirac field is given by

$$H = \int \psi^{\dagger}(-i\alpha.\nabla + m\beta) \psi d^3x. \qquad ...(56)$$

12.9. MAXWELL'S FIELD:

We shall consider the Maxwell's electromagnetic field in the absence of source, charges and currents, i.e., we study free readiation. It can be described by the electric and the magnetic field strength vectors E and B, which satisfy the Maxwell's equations:

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = 0$$

$$\nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} \qquad ...(57)$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}.$$

and

The electromagnetic field, in the relativistic form, is represented by the four potential A_{μ} . The antisymmetric field tensor $F_{\mu\nu}$ is defined by

$$F_{\mu\nu} = \frac{\partial A_{\nu}}{\partial x_{\mu}} - \frac{\partial A_{\mu}}{\partial x_{\nu}} \qquad ...(58)$$

In terms of the components of the field strengths E and B, this can be written as

$$F_{\mu\nu} = \begin{pmatrix} 0 & B_3 & -B_2 & -iE_1 \\ -B_3 & 0 & B_1 & -iE_2 \\ B_2 & -B_1 & 0 & -iE_3 \\ iE_1 & iE_2 & iE_3 & 0 \end{pmatrix} ...(59)$$

The Maxwell's equations (57) can be written in terms of A_{μ} in a very concise form as

$$\Box A_{\mu} = 0 \qquad ...(60)$$

where A_{μ} satisfies

$$\frac{\partial A_{\mu}}{\partial x_{\mu}} = 0 \qquad \dots (61)$$

This eqn. is known as the Lorentz condition.

The electromagnetic field equations are invariant under the gauge transformation of the second kind, defined by:

$$A_{\mu} \rightarrow A'_{\mu} = A_{\mu} - \partial_{\mu} \chi, \qquad ...(62)$$

where Z is an arbitrary complex scalar function, restricted only by

$$\square \chi = 0,$$
 ...(63)

so that the new potential A_{μ} can satisfy the Lorentz condition. Therefore, the potential A_{μ} is not an observable quantity and it is introduced merely to simplify the computations. Only the field tensor $F_{\mu\nu}$ is an observable; i.e., only the electric and magnetic fields are observable. Only those quantities have a physical meaning which are invariant under the transformation (62). This is called gauge invarance,

Now we write down the expression for the Lagrangian density for the electromagnetic field from which we can get the Maxwell's equations as the Euler Lagrange's eqns. The Lagrangian density for a real scalar field with mass 'm' is given by (34) as

$$L = -\frac{1}{2}m^2 \Phi^2_{\alpha} - \frac{1}{2}(\partial_{\mu}\Phi_{\alpha})^2$$

Hence the Lagrangian density for the Maxwell's electromagnetic field (a real vector field) with vanishing rest mass can be written as

$$L = -\frac{1}{2} (\partial_{\mu} A_{\nu})^{2} \dots (64)$$

Klein-Gordon equation with m=0, i.e., the Maxwell's equations $\Box A_{\mu}=0$, for each of the components A_{μ} follows from (64). If we add a four-divergence term to (64) the equation of motion will obviously remain unaltered. Hence we can write $\mathbf{L}=-\frac{1}{4}\left(\partial_{\mu}A_{\nu}-\partial_{\nu}A_{\mu}\right)\left(\partial_{\mu}A_{\nu}-\partial_{\nu}A_{\mu}\right)=-\frac{1}{4}F_{\mu\nu}F_{\mu\nu}=\frac{1}{2}\left(E^{2}-B^{2}\right)$...(65)

This form of the lagrangian has the advantage of being "gauge invariant". Using (65), we can derive the Euler Lagrange's equations as follows:

$$\mathbf{L} = -\frac{1}{4} \left[(\partial_{\mu} A_{\nu})^{2} + \partial_{\nu} A_{\mu} \right]^{2} - 2(\partial_{\mu} A_{\nu}) \left(\partial_{\nu} A_{\mu} \right) \right]$$

$$\therefore \frac{\partial \mathbf{L}}{\partial (\partial_{\alpha} A_{\beta})} = -\frac{1}{4} \left[2\partial_{\mu} A_{\nu} \delta_{\sigma \mu} \delta_{\beta \nu} + 2\partial_{\nu} A_{\mu} \delta_{\alpha \nu} \delta_{\beta \mu} \right.$$

$$\left. - 2\partial_{\mu} A_{\nu} \delta_{\alpha \nu} \delta_{\mu \beta} - 2\partial_{\nu} A_{\mu} \delta_{\sigma \mu} \delta_{\beta \nu} \right] +$$

$$= -\frac{1}{4} \left[4\partial_{\alpha} A_{\beta} - 4\partial_{\beta} A_{\alpha} \right]$$

$$= -(\partial_{\alpha} A_{\beta} - \partial_{\beta} A_{\alpha}) = -F_{\alpha \beta}$$

Hence we have

$$\frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} A_{\mu})} \right) = \frac{\partial}{\partial x_{\mu}} \left(-F_{\mu\nu} \right)$$

Also, we have
$$\frac{\partial \mathbf{L}}{\partial \Lambda_{\mu}} = 0$$
.

Thus the Euler Lagrange's eqns. for (65) are given by

$$\frac{\partial F_{\mu\nu}}{\partial x_{\mu}} = 0 \qquad \dots (66)$$

With the Lorentz condition eqn. (61), this reduces to the M_{ax} -well's eqns. $\Box A_{\mu} = 0$. However, the difficulty with the Lagrangian (65) is that the momentum canonically conjugate to A_4 vanishes,

$$\pi_4 = \frac{\partial L}{\partial \left(\frac{\partial A_4}{\partial I}\right)} = -i \frac{\partial L}{\partial \left(\partial_4 A_4\right)} = -i F_{44} = 0.$$

Therefore, Fermi wrote the Lagrangian as

$$L = -\frac{1}{4} F_{\mu\nu} F_{\mu\nu} - \frac{1}{2} (\partial_{\mu} A_{\mu})^{2} \dots (67)$$

which is relativistically invariant but not gauge invariant due to the presence of $(\partial_{\mu} A_{\mu})^2$ term.

The variation with respect to Ar yields

or

or

$$\frac{\partial}{\partial x_{\mu}} \left[\frac{\partial \mathbf{L}}{\partial (\partial_{\mu} A_{\nu})} \right] = \frac{\partial}{\partial x_{\mu}} \left[-F_{\mu\nu} - \delta_{\mu\nu} \left(\partial_{\lambda} A_{\lambda} \right) \right] = 0$$

$$\Box A_{\nu} - \partial_{\nu} \partial_{\lambda} A_{\lambda} + \partial_{\nu} \partial_{\lambda} A_{\lambda} = 0$$

$$\Box A_{\nu} = 0$$

The Lagrangian (67) actually correspods to (65): the two differ only by a divergence,

The momentum canonically conjugate to A_{μ} , using (65); is given by

$$\pi_{\mu} = -i \frac{\partial \mathbf{L}}{\partial \left(\frac{\partial A_{\mu}}{\partial x_{4}}\right)} = -iF_{\mu,4}$$

$$\therefore \quad \tau_{4} = 0 \text{ and } \pi_{k} = i \left(\frac{\partial A_{k}}{\partial x_{4}} - \frac{\partial A_{4}}{\partial x_{k}}\right)$$

$$= \frac{\partial A_{k}}{\partial t} + \frac{\partial \phi}{\partial x_{k}}$$

 $=-E_{k}\{: \text{ in natural units, } \overrightarrow{E} = \overrightarrow{A} - \nabla \phi\}$ Hence the Hamiltonian density can be written as

$$H = \sum_{\mu=1}^{4} \pi_{\mu} \dot{A}_{\mu} - L$$

$$= \sum_{k=1}^{3} (-E_k) \left(-E_k - \frac{\partial \phi}{\partial x_k} \right) - \mathbf{L}$$

$$= E^2 + \mathbf{E} \cdot \nabla \Phi - \mathbf{L}$$

$$= E^2 + \mathbf{E} \cdot \nabla \Phi - \frac{1}{2} (E^2 - B^2)$$

$$= \frac{1}{2} (E^2 + B^2) + \mathbf{E} \cdot \nabla \Phi \qquad ...(68)$$

And the total Hamiltonian is, therefore, given by:

$$H = \int d^3x \ H = \frac{1}{2} \int (E^2 + B^2) \ d^3x + \int \mathbf{E} \cdot \nabla \Phi \ d^3x \quad ...(69)$$

Integrating the second term by parts,

$$\int \mathbf{E} \cdot \nabla \Phi \, d^3x = -\int (\nabla \cdot \mathbf{E}) \, d^3x + \int a^3x \, \nabla \cdot (\mathbf{E}\Phi)$$

From the Maxwell's eqn. $\nabla E=0$, the first term on the right hand side of above vanishes. Also the second term vanishes, because it can be written as a surface integral using the Gauss theorem and the field strength E and the scalar potential ϕ vanishes at infinity. Therefore,

$$H = \frac{1}{2} \int (E^2 + B^2) \ d^3x \qquad ...(70)$$

this is clearly positive definite and gives the total energy of the field.

12.10. PROCA'S FIELD:

A vector field with nonzero rest mass is known as Proca's Field. The Lagrangian density for this field can be written as

$$\mathbf{L} = -\frac{1}{2} m^2 V_{\mu} V_{\mu} - \frac{1}{2} (\partial_{\mu} V_{\nu})^2 \qquad ...(71)$$

We can write a more appropriate form of Lagrangian density by taking analogy from the Maxwell's Field. We define the antisymmetric field tensor

$$P_{\mu\nu} = \partial_{\mu} V_{\nu} - \partial_{\nu} V_{\nu} \qquad ...(72)$$

and write

$$L = -\frac{1}{2}m^2 V_{\mu}V_{\mu} - \frac{1}{4}F_{\mu\nu}^2 \qquad ...(73)$$

To find the field equations, we have

$$\frac{\partial L}{\partial V_{\mu}} = -m^2 V_{\mu}; \qquad \frac{\partial L}{\partial (\partial_{\mu} V_{\nu})} = -P_{\mu\nu}.$$

Hence the field equations can be written as

$$\partial_{\mu}P_{\mu\nu}=m^2V_{\mu} \qquad ...(74)$$

Differentiating (74), we get

$$\partial_{\nu}\partial_{\mu}P_{\mu\nu}=m^2\partial_{\nu}V_{\mu}$$

Now ∂_{ν} ∂_{μ} is a symmetric tensor and $P_{\mu\nu}$ is an antisymmetric tensor, therefore, their product $\partial_{\nu}\partial_{\mu}P_{\mu\nu}$ vanishes, and hence we get

$$\partial_{\nu}V_{\mu}=0$$
 (: $m\neq 0$) ...(75)

This condition is analogous to the Lorentz condition (61). This must be satisfied by the free Proca field.

The Quanta of the Maxwell's field are the zero mass and one spin well known photons. Their behaviour is described by the Maxwell's equations. Around 1935 it was believed that the Proca's field, on quantization, describes some sort of mesons. Currently, however, we have no evidence for the existence of spin one particle with a nonvanishing rest mass.

PROBLEMS

Problem 1. The energy momentum tensor for fields is defined by

$$T_{\mu\nu} = \sum_{\alpha} \pi_{\mu\alpha} \partial_{\nu} \psi_{\alpha} - L \delta_{\mu\nu} \qquad ...(i)$$

Show that

$$\frac{\partial T_{\mu\nu}}{\partial x_{\mu}} = 0$$

where it is assumed that the field satisfies the Euler lagrange's equation.

(b) Each component of the four vector

$$P_{\nu}(t) = -i \int T_{4\nu} d^3x$$

is constant in time if ψ_{α} vanishes sufficiently rapidly at infinity.

(c) What is the significance of the components of the vector P_{ν} ?

Sol. (a) From (i), we have
$$\frac{\partial T_{\mu\nu}}{\partial x_{\mu}} = \sum_{\alpha} \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \psi_{\alpha})} \right) \partial_{\nu} \psi_{\alpha} + \sum_{\alpha} \frac{\partial L}{\partial (\partial_{\mu} \psi_{\alpha})} \frac{\partial}{\partial x_{\mu}} (\partial_{\nu} \psi_{\alpha})$$

$$- \frac{\partial L}{\partial x_{\nu}} \qquad \left\{ : \pi_{\mu\alpha} = \frac{\partial L}{\partial (\partial_{\mu} \psi_{\alpha})} \right\}$$

Using the Euler Lagrange equations (18), we can write it as

$$\frac{\partial T_{\mu\nu}}{\partial x_{\mu}} = \sum_{\alpha} \frac{\partial L}{\partial \psi_{\alpha}} \partial_{\nu} \psi_{\alpha} + \sum_{\alpha} \frac{\partial L}{\partial (\partial_{\mu} \psi_{\alpha})} \partial_{\mu} (\partial_{\nu} \psi_{\alpha}) - \frac{\partial L}{\partial x_{\nu}} \dots (ii)$$

Now the Lagrangian density L is a function of ψ_{α} and $\partial_{\mu}\psi_{\alpha}$. Therefore,

or

$$\frac{\partial L}{\partial x_{\nu}} = \sum_{\alpha} \frac{\partial L}{\partial \psi_{\alpha}} \partial_{\nu} \psi_{\alpha} + \sum_{\alpha} \frac{\partial L}{\partial (\partial_{\mu} \psi_{\alpha})} \partial_{\nu} (\partial_{\mu} \psi_{\alpha})$$

Since $\partial_{\nu} \partial_{\mu}$ is symmetrical, therefore, $\partial_{\nu} (\partial_{\mu} \psi_{\alpha}) = \partial_{\mu} (\partial_{\nu} \psi_{\alpha})$. Hence we have from (ii) that

$$\frac{\partial T_{\mu\nu}}{\partial x_{\mu}} = 0 \qquad ...(iii)$$

(b) Eqn: (iii) can be written as

$$\frac{\partial T_{4\nu}}{\partial x_4} + \frac{\partial T_{i\nu}}{\partial x_4} = 0$$

Integrating it over the finite space, we get

$$\frac{\partial}{\partial x_4} \int T_{4\nu} d^3x + \frac{\partial}{\partial x_1} \int T_{4\nu} d^3x = 0 \qquad ...(iv)$$

The second integral on the L.H.S. of the above eqn. can be written, by using Gauss Theorem, as

$$\frac{\partial}{\partial x_i} \int T_{i\nu} d^3x = \int \nabla . T_{\nu} d^3x = \int T_{\nu} . dS, \qquad ...(v)$$
surface

where the surface of integration is the infinite surface bounding the entire space. Since the field ψ_{α} vanishes at infinity, therefore, T_{ν} vanishes over the surface at infinity. Thus the right hand side of (v) vanishes and hence we can write from (iv) as

 $\frac{\partial}{\partial x_4} \int T_{4\nu} d^3x = 0$ $-i \frac{\partial}{\partial t} \int T_{4\nu} d^3x = 0 \qquad (\therefore x_4 = it)$

Defining $P_{\nu} = -i \int T_{4\nu} d^3x$, we can write from t as:

$$\frac{\partial P_{\nu}}{\partial t} = 0 \Rightarrow P_{\nu}$$
 is constant in time.

(c) From the definition of $T_{\mu\nu}$, we have

$$T_{44} = \sum_{\alpha} \pi_{\alpha} \dot{\psi}_{\alpha} - L = H,$$

the Hamiltonian density for the field. Therefore,

$$P_4 = -i \int H d^3x = -iE,$$

where E is the total energy of the field.

The first three components of P_{ν} correspond to the conservation of the quantities

$$P_{k} = -i \int T_{4k} d^{3}x$$

$$= \int \pi_{2} \partial_{k} \psi_{\alpha} d^{3}x \qquad ...(vi)$$

These are the three components of the total linear momentum $P = \int \pi_{\alpha} \nabla \psi_{\alpha} d^3x$...(vii)

Hence the vector P_{ν} is the total four energy momen um vector for the field. Its first three components are the components of the total linear momentum of the field and the last component gives the total energy of the field.

Problem 2. The orbital angular momentum for a particle system is defined by

 $L_{ij} = x_i p_j - x_j p_i \qquad \dots (1)$

Taking analogy from it, define the orbital angular momentum for the fields.

Does the orbital angular momentum for the fields remain constant in time? Explain.

Sol. From the last problem, we have the total linear momentum for the fields as

 $P_k = -i \int T_{4k} d^3x = \int \pi_{\alpha} \partial_k \psi_{\alpha} d^3x.$

Hence, we can define the density of the total linear momentum as

$$\mathbf{p}_{k} = -i T_{4k} = \pi_{\alpha} \partial_{k} \psi_{\alpha}. \tag{ii}$$

Thus by taking analogy from (i), we can write the orbital angular momentum density for the field as

$$L_{ij} = x_i P_j - x_i P_i$$

In the tensorial form, it can be written as

$$L_{ij} = -i (x_i T_{4j} - x_j T_{4i})$$
 ...(iii)

Total orbital angular momentum of the field can be found by integrating (iii) over the entire space.

As a generalization of (iii), we can define an angular momentum tensor for the fields as

$$L_{\lambda\mu\nu} = x_{\mu} T_{\lambda\nu} - x_{\nu} T_{\lambda\mu}. \qquad ...(iv)$$

From (iv), we have that

$$\frac{\partial L_{\lambda\mu\nu}}{\partial x_{\lambda}} = \delta_{\mu\lambda} T_{\lambda\nu} + x_{\mu} \frac{\partial T_{\lambda\nu}}{\partial x_{\lambda}} - \delta_{\nu\lambda} T_{\lambda\mu} - x_{\nu} \frac{\partial T_{\lambda\mu}}{\partial x_{\lambda}}$$

$$= T_{\mu\nu} - T_{\nu\mu} \qquad \left\{ \because \frac{\partial T_{\lambda\nu}}{\partial x_{\lambda}} = 0 \right\}$$

$$\neq 0 \text{ in general.} \qquad \dots (v)$$

From (v), we see that $L_{ij} \neq \text{constant}$ in time for the field. This is so, because the spin of the field is not introduced and only the orbital part of the angular momentum is considered. But, if the energy momentum tensor $T_{\mu\nu}$ is symmetric, i.e. $T_{\mu\nu} = V_{\nu\mu}$, then the orbital angular momentum will be a constant in time. Although from the definition, we can not say about the symmetry

of $T_{\mu\nu}$, yet it is always possible to symmetrise the energy momentum by making use of the fact that the addition of a four divergence to the Lagrangian does not affect the field equations. Thus we can say that the orbital angular momentum for the classical field is constant in time.

Problem 3. Show that the Dirac equation in the presence of an electromagnetic field A_{μ} ,

$$[\gamma_{\mu} (\partial_{\mu} - ie A_{\mu}) + m] \psi = 0 \qquad ...(i)$$

can be made invariant under simultaneous gauge transformations on ψ and A_{μ} , and find the connection between the two gauge functions.

Sol. Under the gauge transformation of first kind, ψ changes as

$$\psi \rightarrow \psi' = \psi e^{i\alpha} (x)$$
 ...(ii)

To find the transformed equation, we multiply (i) by $e^{i\alpha}$ (x) from the left

$$e^{i\alpha}$$
 (x) $[\gamma_{\mu} (\partial_{\mu} - ie A_{\mu}) + m] \psi = 0.$...(iii)

Now for an arbitrary function f(x), we have

$$[f(x), \partial_{\mu}] \psi(x) = f(x) \partial_{\mu} \psi - \partial_{\mu} [f(x) \psi(x)]$$

$$= f(x) \partial_{\mu} \psi - f(x) \partial_{\mu} \psi(x) - \partial_{\mu} f(x) \psi(x)$$

$$= -\partial_{\mu} f(x) \cdot \psi(x)$$

$$\Rightarrow [f(x), \partial_{\mu}] = -\partial_{\mu} f(x)$$

$$\vdots [e^{i\alpha}(x), \partial_{\mu}] = -ie^{i\alpha} (\partial_{\mu} \alpha)$$

$$\Rightarrow e^{i\alpha} \partial_{\mu} = \partial_{\mu} e^{i\alpha} - ie^{i\alpha} (\partial_{\mu} \alpha).$$

Using it, we can write (iii) as

$$[\gamma_{\mu} (\partial_{\mu} - ie A_{\mu} - i \partial_{\mu} x) + m] e^{i\alpha} \psi = 0$$

$$[\gamma_{\mu} (\partial_{\mu} - ie A_{\mu} - i \partial_{\mu} x) + m] \psi' = 0$$
(iv)

Thus the Dirac eqn. (i) is not invariant under the gauge transformation of first kind and the term $i \partial_{\mu} x$ spoils its invariance.

Applying the gauge transformation of second kind

$$A_{\mu} \rightarrow A'_{\mu} = A_{\mu} - \partial_{\mu} \chi$$
...(v)

to (iv), we obtain

or

For the invariance, we should have

$$ie \partial_{\mu} \chi - i \partial_{\mu} \alpha \equiv 0$$

or $\alpha = e\chi$(v)

Choosing $\alpha = e \chi$ we see that the eqn. (i) is invariant under the simultaneous gauge transformations on ψ and A_{μ} (vi) gives the connection between the two gauge functions.

Problem 4. The Lagrangian density for the Dirac field in

interaction with the e.m. field is given by

 $\mathbf{L} = -\bar{\psi} \left[\gamma_{\mu} \left(\partial_{\mu} - ie A_{\mu} \right) + m \right] \psi. \tag{i}$

Show that it can be made invariant under simultaneous gauge transformations of the first and second kind. Also show that the charge conservation follows from the invariance under the combined gauge transformations.

Sol. Exactly on the lines of the last problem, we can show that for $\alpha = eX$; L is invarient under the simultaneous gauge transformations of first and second kind.

Now, to see the consequence of this invariance we write the Lagrangian (i) as L (ψ , ψ , A_{ν} , $\partial_{\mu}\psi$, $\partial_{\mu}\psi$, $\partial_{\mu}A_{\nu}$). The infinitesimal elements of the gauge transformations are given as

$$A_{\mu} \rightarrow A_{\mu} - \partial_{\mu} \chi \Rightarrow \delta A_{\mu} = -\partial_{\mu} \chi,$$

$$\psi \rightarrow \exp. (ie\chi) \psi = (1 + ie\chi) \psi \Rightarrow \delta \psi = ie\chi\psi,$$

$$\overline{\psi} = \exp. (-ie\chi) \overline{\psi} = (1 - ie\chi) \overline{\psi} \Rightarrow \delta \overline{\psi} = -ie\chi\overline{\psi} ...(ii)$$

and

The change in L due to these variation $\delta \psi$, $\delta \overline{\psi}$ and δA_v is given by

$$\begin{split} \partial L &= \frac{\partial L}{\partial \psi} \, \delta \psi + \frac{\partial L}{\partial \bar{\psi}} \, \delta \bar{\psi} + \frac{\partial L}{\partial A_{\nu}} \, \delta A_{\nu} + \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \delta \left(\partial_{\mu} \psi \right) \\ &\quad + \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \delta \left(\partial_{\mu} \bar{\psi} \right) + \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \delta \left(\partial_{\mu} A_{\nu} \right) \\ &\quad = \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \right) \, \delta \psi + \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \right) \, \delta \bar{\psi}. \\ &\quad + \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \right) \, \delta A_{\nu} + \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \partial_{\mu} (\delta \psi) + \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \partial_{\mu} \left(\delta \bar{\psi} \right) \\ &\quad + \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \partial_{\mu} \left(\delta A_{\nu} \right) \qquad \qquad \{ \text{Using field equations} \} \\ &\quad = \frac{\partial}{\partial x_{\mu}} \left[\frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \delta \psi + \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \delta \psi + \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \delta A_{\nu} \right] \\ &\quad = \frac{\partial}{\partial x_{\mu}} \left[ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \chi \psi - ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \chi \bar{\psi} - \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \partial_{\nu} \chi \right] \\ &\quad = \frac{\partial}{\partial x_{\mu}} \left[ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \chi \psi - ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \chi \bar{\psi} - \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \partial_{\nu} \chi \right] \\ &\quad = \frac{\partial}{\partial x_{\mu}} \left[ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \chi \psi - ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \chi \bar{\psi} - \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \partial_{\nu} \chi \right] \\ &\quad = \frac{\partial}{\partial x_{\mu}} \left[ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \, \chi \psi - ie \, \frac{\partial L}{\partial \left(\partial_{\mu} \bar{\psi} \right)} \, \chi \bar{\psi} - \frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu} \right)} \, \partial_{\nu} \chi \right] \end{aligned}$$

Since the Lagrangian L is is invariant, δL must be zero. Thus we have

$$\frac{\partial}{\partial x_{\mu}} \left[ie \frac{\partial L}{\partial (\partial_{\mu} \psi)} \chi \psi - ie \frac{\partial L}{\partial (\partial_{\mu} \psi)} \chi \overline{\psi} - \frac{\partial L}{\partial (\partial_{\mu} A_{\nu})} \partial_{\nu} \chi \right] = 0 \dots (iii)$$

Noting that $(\partial_{\mu}A_{\nu})$ occurs only in the free e.m. part, $-\frac{1}{4}F_{\mu\nu}$ $F_{\mu\nu}$, of the Lagrangian, we have

$$\frac{\partial L}{\partial \left(\partial_{\mu} A_{\nu}\right)} = -F_{\mu\nu}$$

Thus the last term in (iii) gives

$$\frac{\partial}{\partial x_{\mu}} \left[-F_{\mu\nu} \partial_{\nu} \chi \right] = - \frac{\partial F_{\mu\nu}}{\partial x_{\mu}} \left(\partial_{\nu} \chi \right) - F_{\nu\nu} \partial_{\mu} \partial_{\nu} \chi$$

Since $F_{\mu\nu}$ is antisymmetric and $(\partial_{\mu}\partial_{\nu})$ is a symmetric tensor, therefore, their product vanishes. Hence we get

$$\frac{\partial}{\partial x_{\mu}} \left[-F_{\mu\nu} \partial_{\nu} \chi \right] = -\frac{\partial F_{\mu\nu}}{\partial x_{\mu}} \left(\partial_{\nu} \chi \right)$$

$$= -j_{\nu} \left(\partial_{\nu} \chi \right) \left\{ : \text{ the current density } j_{\nu} = \frac{\partial F_{\mu\nu}}{\partial x_{\mu}} \right\}$$

Using it, we can write (iii) as:

$$j_{\mu} \left(\partial_{\mu} \chi \right) + \partial_{\mu} \left[ie \chi \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \psi - ie \chi \frac{\partial L}{\partial \left(\partial_{\mu} \overline{\psi} \right)} \overline{\psi} \right] = 0.$$

$$\left[j_{\mu} - ie \frac{\partial L}{\partial \left(\partial_{\mu} \overline{\psi} \right)} \overline{\psi} - \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \psi \right) \right] \partial_{\mu} \chi$$

$$- \partial_{\mu} \left[ie \left(\frac{\partial L}{\partial \left(\partial_{\mu} \overline{\psi} \right)} \overline{\psi} - \frac{\partial L}{\partial \left(\partial_{\mu} \psi \right)} \psi \right) \right] \chi = 0.$$

Since X and $\partial_{\mu}X$ are arbitrary, it follows that

$$j_{\mu} = ie \left(\frac{\partial L}{\partial (\partial_{\mu} \overline{\psi})} \overline{\psi} - \frac{\partial L}{\partial (\partial_{\mu} \psi)} \psi \right) \qquad ...(iv)$$

and

or

$$\partial_{\mu} \left[ie \left(\frac{\partial L}{\partial (\partial_{\mu} \overline{\psi})} \overline{\psi} - \frac{\partial L}{\partial (\partial_{\mu} \psi)} \psi \right) \right] \equiv \partial_{\mu} j_{\mu} = 0 \qquad (v)$$

Eqn. (iv) gives the current density j_{μ} from the Lagrangian density L and the eqn. (v) shows that this current satisfies the eqn. of continuity.

Eqn. (v) defines a constant of motion for the gauge transformation $-i \int j_4 d^3x$. This constant corresponds to the total charge of the field.

$$Q = e \int \left(\frac{\partial L}{\partial (\partial_4 \overline{\psi})} \, \overline{\psi} - \frac{\partial L}{\partial (\partial_4 \psi)} \, \psi \, \right) \, d^3 x$$
the charge correspond to (Vi)

Thus the charge conservation follows as a consequence of the invariance under the combined gauge transformations.

Problem 5. Show that the invariance under translation leads to the conservation of energy and the momentum for the scalar field, defined by the Lagrangian density $L(\varphi_{\alpha}, \partial_{\mu}, \varphi_{\alpha})$.

Sol. A translation is described as

$$x_{\mu} \rightarrow x_{\mu}' = x_{\mu} + \alpha_{\mu}$$
 ...(i)

The change in the Lagrangian under (i) is given by

 $\delta L = L (x_{\parallel} + \alpha_{\mu}) - L (x_{\parallel})$

For an infinitesimal translation, we can take α_{μ} as an arbitrary infinitesimal constant. Thus expanding $L(x_{\mu} + \alpha_{\mu})$ by Taylor's series and retaining only the first order term we have

$$\delta L = \alpha_{\mu} \frac{\partial L}{\partial x_{\mu}} = \delta_{\mu\nu} \alpha_{\nu} \frac{\partial L}{\partial x_{\nu}} \qquad ...(ii)$$

Also, the change in p_{α} under (i) can be written as:

$$\delta \varphi_{\alpha} = \varphi_{\alpha} (x_{\mu} + \alpha_{\mu}) - \varphi_{\alpha} (x_{\mu})$$

$$= \alpha_{\mu} \frac{\partial \varphi_{\alpha}}{\partial x_{\mu}} = \alpha_{\mu} \partial_{\mu} \varphi_{\alpha} \qquad ... (iii)$$

Therefore, the change in L can also be written as:

$$\delta L = \sum_{\alpha} \left(\frac{\partial L}{\partial \varphi_{\alpha}} \delta \varphi_{\alpha} + \frac{\partial L}{\partial (\partial_{\mu} \varphi_{\alpha})} \delta (\partial_{\mu} \varphi_{\alpha}) \right)$$

$$= \sum_{\alpha} \left[\frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \varphi_{\alpha})} \right) \delta \varphi_{\alpha} + \frac{\partial L}{\partial (\partial_{\mu} \varphi_{\alpha})} \delta (\partial_{\mu} \varphi_{\alpha}) \right]$$

{Using Euler Lagrange eqn.}

$$= \sum_{\alpha} \left[\frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \varphi_{\alpha})} \right) \cdot \alpha_{\nu} \partial_{\nu} \varphi_{\alpha} + \frac{\partial L}{\partial (\partial_{\mu} \varphi_{\alpha})} \partial_{\mu} (\alpha_{\nu} \partial_{\nu} \varphi_{\alpha}) \right]$$

{Using (iii) and $\delta (\partial_{\mu} \varphi_{\alpha}) = \partial_{\mu} (\delta \varphi_{\alpha})$ }

or
$$\delta L = \alpha_v \sum_{\alpha} \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial (\partial_{\mu} \varphi_{\alpha})} \partial_{\nu} \varphi_{\alpha} \right)$$
 ...(iv)

From (ii) and (iv) we have

$$\delta_{\mu\nu}\alpha_{\nu}\frac{\partial L}{\partial x_{\mu}} = \alpha_{\nu}\sum_{\alpha}\frac{\partial}{\partial x_{\mu}}\left(\frac{\partial L}{\partial(\partial_{\mu}\varphi_{\alpha})}\partial_{\nu}\varphi_{\alpha}\right)$$

or
$$\frac{\partial}{\partial x_{\mu}} \left[\sum_{\alpha} \frac{\partial L}{\partial (\partial_{\mu} p_{\alpha})} \partial_{\nu} p_{\alpha} - L \delta_{\mu\nu} \right] = 0$$

or
$$\frac{\partial T_{\mu\nu}}{\partial x_{\mu}} = 0 \qquad \dots (v)$$

 $T_{\mu\nu}$ is the energy momentum tensor. We have seen that eqn. (v) implies the conservation of energy and momentum.

Problem 6. The following one dimensional Lagrangian density is appropriate for a continuous acoustic field

$$\mathbf{L} = \frac{1}{2} \, \rho \left(\frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} \, T \left(\frac{\partial \phi}{\partial x} \right)^2 \qquad \dots (i)$$

where ϕ is the deviation from equilibrium position and ρ and T are positive constants. Calculate the Hamiltonian and obtain the equation of motion. (Assume the length of the medium to be L).

Sol. The equation of motion is given by

$$\frac{\partial L}{\partial \varphi} - \frac{\partial}{\partial x_{\mu}} \left(\frac{\partial L}{\partial \left(\frac{\partial}{\partial x_{\mu}} \right)} \right) = 0 \qquad ...(ii)$$

For a one dimensional field, it reduces to

$$\frac{\partial \mathbf{L}}{\partial \varphi} - \frac{\partial}{\partial x} \left(\frac{\partial \mathbf{L}}{\partial \left(\frac{\partial \phi}{\partial x} \right)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathbf{L}}{\partial \left(\frac{\partial \phi}{\partial t} \right)} \right) = 0 \qquad \dots \text{(iii)}$$

From (i) we have

$$\frac{\partial \mathbf{L}}{\partial \phi} = 0$$
; $\frac{\partial \mathbf{L}}{\partial \phi} = \rho \dot{\phi}$ and $\frac{\partial \mathbf{L}}{\partial \left(\frac{\partial \phi}{\partial x}\right)} = -T\left(\frac{\partial \phi}{\partial x}\right)$.

Putting these values in (iii), we get the eqn. of motion as:

$$T \frac{\partial^2 \phi}{\partial x^2} - \rho \frac{\partial^2 \phi}{\partial t^2} = 0 \qquad ...(iv)$$

Now, the canonical conjugate momentum density is given by

$$\pi \equiv \frac{\partial L}{\partial \dot{\phi}} = \rho \left(\frac{\partial \phi}{\partial t} \right)$$

Therefore, the Hamiltonian density is given as:

$$H = \pi \dot{\phi} - L = \frac{1}{2} \rho \dot{\phi}^2 + \frac{1}{2} T \left(\frac{\partial \phi}{\partial x} \right)^2$$

And the Total Hamiltonian is given by

$$H = \frac{1}{2}\rho \int_0^L \dot{\phi}^2 dx + \frac{1}{2}T \int_0^L \left(\frac{\partial \phi}{\partial x}\right)^2 dx \qquad \dots (v)$$

Problem 7. Find the Hamiltonian density for the free Proca field and show that it is positive definite.

Sol. The Lagrangian density for the free Proca field is given by

$$L = -\frac{1}{4} P_{\mu\nu}^2 - \frac{1}{2} m^2 V_{\mu} V_{\nu} \qquad ...(i)$$

where

$$P_{\mu\nu} = \partial_{\mu} V_{\nu} - \partial_{\nu} V_{\mu} \qquad ...(ii)$$

The conjugate momentum density is given by

$$\pi_{\mu} = \frac{\partial \mathbf{L}}{\partial (\dot{\mathbf{V}}_{\mu})} = -iP_{\mu 4}$$

 $\pi_4 = 0 \text{ and } \pi_k = -iP_{k4}$

Hence the Hamiltonian density is given as:

$$H = \pi_k \dot{V}_k - L = -iP_{k4}\dot{V}_k + \frac{1}{4}P_{\mu\nu}^2 + \frac{1}{2}m^2V_{\mu}^2 \qquad ... \text{(iii)}$$

Now,

Day

$$P_{\mu\nu}^{2} = P_{kl}^{2} + P_{\mu}^{2} + P_{4\mu}^{2}$$

$$= 2 (\nabla \times \mathbf{V})^{2} + 2 (P_{k4})^{2} \qquad \{ : P_{44} = 0 \}$$

It is clearly positive definite.

Problem 8. The Lagrangian density for a massive vector field interacting with a four vector density j_{μ} is given by

$$\mathbf{L} = -\left[\frac{1}{4} \left(\frac{\partial \phi_{\nu}}{\partial x_{\mu}} - \frac{\partial \phi_{\mu}}{\partial x_{\nu}}\right) \left(\frac{\partial \phi_{\nu}}{\partial x_{\mu}} - \frac{\partial \phi_{\mu}}{\partial x_{\nu}}\right) + \frac{1}{2} m^{2} \dot{\phi}_{\mu} \phi_{\mu}\right] + j_{\mu} \phi_{\mu};$$

obtain the field equations. Also show that $\frac{\partial \phi_{\mu}}{\partial x_{\mu}} = 0$ only if $\partial_{\mu} j_{\mu} = 0$,

Sol. To find the field equations, we have

$$\frac{\partial \mathbf{L}}{\partial \phi_{\mu}} = -m^2 \phi_{\mu} + j_{\mu}$$

and

$$\frac{\partial L}{\partial (\partial_{\mu}\phi_{\nu})} = -\left(\frac{\partial \phi_{\nu}}{\partial x_{\mu}} - \frac{\partial \phi_{\mu}}{\partial x_{\nu}}\right)$$

Hence the field equations are given as

$$\frac{\partial}{\partial x_{\nu}} \left(\frac{\partial \phi_{\nu}}{\partial x_{\mu}} - \frac{\partial \phi_{\mu}}{\partial x_{\nu}} \right) = m^{2} \phi_{\mu} - j_{\mu}. \tag{i}$$

Differentiating (i); we get

$$\frac{\partial}{\partial x_{\mu}} \cdot \frac{\partial}{\partial x_{\nu}} \left(\frac{\partial \phi_{\nu}}{\partial x_{\mu}} - \frac{\partial \phi_{\mu}}{\partial x_{\nu}} \right) = m^{2} \frac{\partial \phi_{\mu}}{\partial x_{\mu}} - \frac{\partial j_{\mu}}{\partial x_{\mu}}$$

$$m^{2} \frac{\partial \phi_{\mu}}{\partial x_{\mu}} = \frac{\partial j_{\mu}}{\partial x_{\mu}}$$
...(ii)

or

{: The L.H.S. being the product of a symmetric and an antisymmetric tensor vanishes}.

From (ii) it is clear that $\partial_{\mu}\phi_{\mu}=0$ only if $\partial_{\mu}j_{\mu}=0$.

Problem 9. What quantity is conserved due to invariance of the fields under infinitesimal rotation. Explain the significance of various terms of this quantity.

Sol. Rotations in four-dimensional space are proper Lorentz transformations and can be characterized by the co-ordinate transformations

$$x_{\mu} \to x'_{\mu} = a_{\mu \nu} x_{\nu} \; ; \; x_{\nu} = a_{\mu \nu} x'_{\mu} \qquad ...(i)$$

where the transformation coefficients satisfy the relation

$$a_{\mu\nu} a_{\mu\lambda} = \delta_{\nu\lambda}$$
 ...(ii)

Similarly, the field variables transform as

$$\psi_{\alpha}(x) \rightarrow \psi'_{\alpha}(x') = b_{\alpha\beta} \psi_{\beta}(x) \qquad ...(iii)$$

For infinitesimal transformations, $a_{\mu\nu}$ will deviate only slightly from the unit matrix and we can write

$$a_{\mu\nu} = \delta_{\mu\nu} + \alpha_{\mu\nu}$$

αμν is infinitesimal. Using it, eqn. (ii) can be written as

$$(\delta_{\mu\nu} + \alpha_{\mu\nu}) (\delta_{\mu\lambda} + \alpha_{\mu\lambda}) = \delta_{\nu\lambda}$$
.

Retaining only the first order term in a, it can be written as

$$\delta_{\nu\lambda} + \alpha_{\lambda\nu} + \alpha_{\nu\lambda} = \delta_{\nu\lambda} \Rightarrow \alpha_{\lambda\nu} + \alpha_{\nu\lambda} = 0$$

i.e., a is an antisymmetric tensor.

Analogously, for (iii), we can write

$$b_{\alpha\beta} = \delta_{\alpha\beta} + \beta_{\alpha\beta}, \ \beta_{\alpha\beta} = I^{\mu\nu}_{\alpha\beta} \alpha_{\mu\nu}, \qquad ...(iv)$$

the transformation coefficients I are antisymmetric in the indices α and β .

Thus, the change $\delta\psi_{\alpha}$ in ψ_{α} under the rotation (iv) can be written as

$$\delta\psi_{\alpha} = \psi'_{\alpha}(x') - \psi_{\alpha}(x) = I^{\mu\nu}_{\alpha\beta}\beta_{\mu\nu}\psi_{\beta}. \qquad ...(v)$$

In case of rotation, δ and ∂_{μ} do not commute as shown below:

$$\delta (\partial_{\mu}\psi_{\alpha}) = \partial'_{\mu}\psi_{\alpha}' (x') - \partial_{\mu}\psi_{\alpha} (x)$$

$$= \partial'_{\mu} [\delta\psi_{\alpha} + \psi_{\alpha}] - \partial_{\mu}\psi_{\alpha}$$

$$= \frac{\partial}{\partial x_{\nu}} [\psi_{\alpha} + \delta\psi_{\alpha}] \frac{\partial x_{\nu}}{\partial x'_{\mu}} - \partial_{\mu}\psi_{\alpha}$$

$$= [\partial_{\nu}\psi_{\alpha} + \partial_{\nu} (\delta\psi_{\alpha})] (\delta_{\mu\nu} + \alpha_{\mu\nu}) - \partial_{\mu}\psi_{\alpha}$$

$$= \partial_{\mu}\psi_{\alpha} + \partial_{\mu} (\delta\psi_{\alpha}) + \alpha_{\mu\nu}\partial_{\nu}\psi_{\alpha} - \partial_{\mu}\psi_{\alpha}$$

$$\vdots \delta (\partial_{\mu}\psi_{\alpha}) = \alpha_{\mu\nu}\partial_{\nu}\psi_{\alpha} + \partial_{\mu} (\delta\psi_{\alpha}). \qquad ...(vi)$$

For an infinitesimal rotation, the change, δL , in the Lagrangian density is given by

$$\begin{split} \delta \mathsf{L} &= \frac{\partial \mathsf{L}}{\partial \psi_{\alpha}} \ \delta \psi_{\alpha} + \frac{\partial \mathsf{L}}{\partial \left(\delta_{\mu} \psi_{\alpha} \right)} \ \delta \left(\partial_{\mu} \psi_{\alpha} \right) \\ &= \frac{\partial \mathsf{L}}{\partial \overline{\psi}_{\alpha}} I_{\alpha\beta}^{\mu\nu} \ \alpha_{\mu\nu} \psi_{\beta} + \frac{\partial \mathsf{L}}{\partial \left(\partial_{\lambda} \psi_{\alpha} \right)} \left[\alpha_{\mu\nu} \ \partial_{\nu} \psi_{\alpha} + \partial_{\lambda} \left(I_{\alpha\beta}^{\mu\nu} \ \alpha_{\mu\nu} \psi_{\beta} \right) \right]^{*} \\ &= \frac{\partial}{\partial x_{\lambda}} \left(\frac{\partial \mathsf{L}}{\partial \left(\partial_{\lambda} \psi_{\alpha} \right)} \right) I_{\alpha\beta}^{\mu\nu} \alpha_{\mu\nu} \psi_{\beta} + \frac{\partial \mathsf{L}}{\partial \left(\partial_{\lambda} \psi_{\nu} \right)} \\ &\times \left[\alpha_{\mu\nu} \ \partial_{\nu} \psi_{\alpha} + \partial_{\lambda} \left(I_{\alpha\beta}^{\mu\nu} \ \alpha_{\mu\nu} \psi_{\beta} \right) \right] \\ &= \frac{\partial}{\partial x_{\lambda}} \left[\left(\frac{\partial \mathsf{L}}{\partial \left(\partial_{\lambda} \psi_{\alpha} \right)} \right) I_{\alpha\beta}^{\mu\nu} \ \alpha_{\mu\nu} \psi_{\beta} \right] + \alpha_{\mu\nu} \left[T_{\mu\nu} + \delta_{\mu\nu} \ \mathsf{L} \right]. \end{split}$$

As $\alpha_{\mu\nu}$ is an antisymmetric tensor, its propuct with the symmetric tensor $\delta_{\mu\nu}$ vanishes. Also, the energy momentum tensor $T_{\mu\nu}$ can be written as

$$T_{\mu\nu} = \frac{T_{\mu\nu} + T_{\nu\mu}}{2} + \frac{T_{\mu\nu} - T_{\nu\mu}}{2}.$$

The first term on the r.h.s. is symmetric and therefore, its product with $\alpha_{\mu\nu}$ vanishes. Thus the change δL can be written as

$$\delta \mathbf{L} = 2 \frac{\partial}{\partial x_{2}} \left[\frac{\partial \mathbf{L}}{\partial (\partial_{\lambda} \psi_{\alpha})} I_{\alpha\beta}^{\mu\nu} \alpha_{\mu\nu} \psi_{\beta} \right] + \alpha_{\mu\nu} \frac{\partial}{\partial x_{\lambda}} \left[x_{\mu} T_{\lambda\nu} - x_{\nu} T_{\lambda\mu} \right].$$

Since the Lagrangian is invariant under the infinitesimal rotation, this change in L must be zero.

$$\therefore \partial_{\lambda} \left[(x_{\mu} T_{\lambda \nu} - x_{\nu} T_{\lambda \mu}) + 2 \frac{\partial L}{\partial (\partial_{\lambda} \psi_{\alpha})} I^{\mu \nu}_{\alpha \beta} \psi^{\beta} \right] = 0 \qquad ...(vii)$$

$$\{ : \alpha_{\mu \nu} \text{ is arbitrary} \}$$

From (vii), we see that the quantity

$$f_{\lambda,\mu\nu} = (x_{\mu}T_{\lambda\nu} - x_{\nu}T_{\lambda,\mu}) + 2\frac{\partial L}{\partial (\partial_{\lambda}\psi_{\alpha})} I_{\alpha\beta}^{\mu\nu} \psi_{\beta} \qquad ...(viii)$$

is conserved. The term in the bracket on the r.h.s. is the orbital angular momentum density Lypy. The second term

$$S_{\lambda\mu\nu} = 2 \frac{\partial L}{\partial (\partial_{\lambda}\psi_{\alpha})} I^{\mu\nu}_{\alpha\beta} \psi_{\beta},$$

in independent of any point of reference and it is related to some intrinsic property of the field. We call it the *spin angular momentum density*. Thus $J_{\lambda\mu\nu}$ is the total angular momentum density of the field which is an invariant quantity.

^{*}We have change the index μ by λ in order to avoid the repetition of the indices. By changing a free index by another one whichdoes not appear already in the expression, the expression remains unchanged,

Problem 10. The matrix I for the Dirac field is given by

$$I_{\alpha\beta}^{\mu\nu} = \frac{i}{4} (\sigma_{\mu\nu})_{\alpha\beta}.$$

Find the total spin for the Dirac field.

Hint: The Lagrangian density of the Dirac field is

$$L = -\psi_{\alpha} \left(\gamma_{\mu} \partial_{\mu} + m \right) \psi_{\alpha}.$$

$$\therefore S_{\lambda_{\mu}\nu} = 2 \frac{\partial L}{\partial \left(\partial_{\lambda} \psi_{\alpha} \right)} I_{\alpha\beta}^{\mu\nu} \psi_{\beta} = -2 \left(\overline{\psi} \gamma_{\lambda} \right)_{\alpha} \cdot \frac{i}{4} \left(\sigma_{\mu\nu} \right)_{\alpha\beta} \psi_{\beta}$$

$$= -\frac{i}{2} \overline{\psi} \gamma_{\lambda} \sigma_{\mu\nu} \psi$$

The total spin of the Dirac field is now given by

$$S = \int L_{4P\nu} d^3x = \frac{1}{2} \int \psi' \stackrel{\rightarrow}{\sigma} \psi d^2x$$

In the last chapter it has been shown that the classical fields are dynamical systems described in terms of the field function $\psi(\mathbf{x}, t)$, which play the role of the generalized coordinates for the fields. Like any other dynamical system, fields possess the energy, momentum and angular momentum etc., which are built up from the field function $\psi(\mathbf{x}, t)$. Similar to the case of classical particle systems; fields obey the Euler Lagrange's equations of motion, which are exactly similar to the Lagrange's equations for a system of particles. The role of classical canonical variables q_i and p_i is played by the field function $\psi(\mathbf{x}, t)$ and canonical conjugate momentum $\pi(\mathbf{x}, t)$. Therefore, like classical particle systems, fields should also exhibit quantum properties, if we want to study them on a micro-scale. Hence we must develop a quantum theory for the fields.

Now we know that the quantum mechanics can be developed from the classical particle mechanics by replacing the canonical variables q_i and p_i by the corresponding hermitian operators, in accordance with the correspondance principle. The equation of motion for these operators is the Heisenberg's equation. The operators q_i and p_i satisfy the following commutation relations:

$$[q_i, q_j] = [p_i, p_j] = 0$$
 and $[q_i, p_j] = i\hbar \delta_{ij}$,

which in terms of natural units ($\hbar = c = 1$) can be written as:

$$[q_i q_j] = [p_i, p_j] = 0$$
, and $[q_i, p_j] = i\delta_{ij}$...(1)

Making use of the above analogies between the classical systems and the classical fields, and that between classical canonical variables and the corresponding quantum mecanical operators, we can develop the quantum theory of fields by defining quantum mechanical operators for the generalized coordinates $\psi(x, t)$ and the canonical momenta $\pi(x, t)$ for the fields. The analogy of q_i and p_i with $\psi(x, t)$ and $\pi(x, t)$ suggests that we can choose the quantum coordinates for the fields as:

^{*}The quantization of fields follows directly from the classical field.

Hence the readers should master the elements of the classical field.

$$[\psi(\mathbf{x}, t), \psi(\mathbf{x}', t)] = [\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = 0 \qquad ...(2a)$$

$$[\psi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = i\delta^{\circ}(\mathbf{x} - \mathbf{x}') \qquad ...(2b)$$

Thus we see that in the quantization of a field; the spacetime field functions $\psi(x, t)$, describing the classical field, become operators. While operated on their eigenfunctions, they give the dynamical observables of the field as the eigenvalues. Thus the field quantization is also known as the second quantization.

In the commutation rules (2), the time parameter of all the variables is the same and hence these are known as equal time commutators. Since the fields are continuous system, therefore, we have used the three dimensional Dirac delta function δ^3 ($\mathbf{r}-\mathbf{r}'$) in place of the Kronecker delta δ_{ij} .

For the cases where the field have more than one component, we write the commutation rules (2) as:

$$[\psi_{\alpha}(\mathbf{x},t),\psi_{\beta}(\mathbf{x}',t)] = [\pi_{\alpha}(\mathbf{x},t),\pi_{\beta}(\mathbf{x}',t)] = 0 \qquad ...(3a)$$

$$[\psi_{\alpha}(\mathbf{x},t),\pi_{\beta}(\mathbf{x}',t)] = i\delta_{\alpha\beta}\delta^{3}(\mathbf{x}-\mathbf{x}') \qquad ...(2b)$$

We shall see shortly that a quantized field represents a system of particles and the interaction between two system of particles then becomes the problem of the interaction between two quantized fields. As an example, the scattering of photons and electrons (Compton Effet), in field theory will be a problem of interaction of a quantized Maxwell's field and a quantized Dirac field. In many interactions, particles are created and destroyed. Thus we need to develop a theory in which these processes are accomodated. Here we shall be quantizing the free fields only i.e., the field without any interaction.

13.1. QUANTIZATION OF REAL SCALAR FIELD:

We have introduced the commutation relations, the field operators should satisfy in the quantum limit. Now we study the consequences of imposing these quantum conditions on the real scalar field ϕ , since it is the simplest of all the fields. We shall work in the Schroedinger picture so that our field operator are time-independent.

The Hamiltonian density for the real scalar classical field is given by (eqn. (37) of last chapter)

$$H = \frac{1}{2} \left[\pi^2 + (\nabla \phi)^2 + m^2 \phi^2 \right]$$

Hence the classical total Hamiltonian is given by

$$H = \int d^3x \cdot \frac{1}{2} \left[\pi^2 + (\nabla \phi)^2 + m^2 \phi^2 \right] \tag{4}$$

In order to find out the physical consequence of the commutation relations for the field operators, and to perform practical calculations, it is most convenient to use Fourier expansions of the field variables $\phi(x)$ and $\pi(x)$ in the momentum space as:

$$q(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} q_k e^{i\mathbf{k} \cdot \mathbf{x}}$$

$$\pi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} p_k e^{-i\mathbf{k} \cdot \mathbf{x}}$$

$$\dots(5)$$

The system is assumed to be in a large box of Volume $V=L^2$, with allowed (discrete) values of the components of k given by:

$$k_x = \frac{2\pi n_x}{L}$$
 etc. with n_x integer.

Summation in (5) is taken over all the allowed values of the vector k. The choice of minus sign in the exponent of $\pi(x)$ is delibrate; it leads to a simplification, as we shall see shortly.

Since ϕ and π are real functions at the classical level. the corresponding operators must be hermitian, i.e.,

$$\phi \dagger(\mathbf{x}) = \phi(\mathbf{x})$$
 and $\pi \dagger(\mathbf{x}) = \pi(\mathbf{x})$

Using (5) we get from these conditions that

$$\frac{1}{\sqrt{(V)}} \sum_{k} q_{i} \dagger e^{-i\mathbf{k}.\mathbf{X}} = \frac{1}{\sqrt{(V)}} \sum_{k} \mathbf{q}_{k} e^{i\mathbf{k}.\mathbf{X}}$$

$$= \frac{1}{\sqrt{(V)}} \sum_{k} q_{-k} e^{-i\mathbf{k}.\mathbf{X}}$$

$$\Rightarrow q_{k}\dagger = q_{-k}$$
 and similarly $p_{k}\dagger = p_{-k}$...(6)

The coefficients q_k and p_k are the dynamical variables on the same footing as the position and the momentum coordinates. In fact, assuming the commutation rules (1) for q_k and p_k we can easily compute the commutator of ϕ and π :

$$[\phi(\mathbf{x}), \pi(\mathbf{x}')] = \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

$$= \sum_{k} [q_k, p_{k'}] e^{i\mathbf{k} \cdot \mathbf{x} - i\mathbf{k}' \cdot \mathbf{x}'}$$

which in the limit $V \rightarrow \infty$, yields

$$[\phi(x), \pi(x')] = i\delta^{3}(x - x') \qquad ...(7)$$
It it exactly the commutation relation (2b).

Alternatively, if we know the commutation rules (2), the commutation rules for q_k 's and p_k 's can be obtained by a procedure which is inverse of that which led to eqn. (7).

Multiplying the first and the second of eqns. (5) by $\frac{1}{\sqrt{(V)}}e^{-i\mathbf{k}.\mathbf{x}}$ and $\frac{1}{\sqrt{(V)}}e^{-i\mathbf{k}.\mathbf{x}}$, respectively, and integrating over the volume V we get the inverse formulae

$$q_{k} = \frac{1}{\sqrt{(V)}} \int d^{3}x \quad \phi(\mathbf{x}) \quad e^{-i\mathbf{k}.\mathbf{x}}$$

$$p_{k} = \frac{1}{\sqrt{(V)}} \int d^{3}x \quad \pi(\mathbf{x}) \quad e^{i\mathbf{k}.\mathbf{x}}$$

$$\therefore [q_{k}, p_{k}'] = \frac{1}{V} \iint d^{3}x d^{3}x' \quad [\phi(\mathbf{x}), \pi(\mathbf{x}')] \quad e^{i\mathbf{k}'.\mathbf{x}' - i\mathbf{k}.\mathbf{x}}$$

$$= \frac{i}{V} \iint d^{3}x d^{3}x' \quad \delta^{3} \quad (\mathbf{x} - \mathbf{x}') \quad e^{i\mathbf{k}'.\mathbf{x}' - i\mathbf{k}.\mathbf{x}}$$

$$= \frac{i}{V} \iint d^{3}x \quad e^{i(\mathbf{k}' - \mathbf{k}).\mathbf{x}} = i\delta_{kk'} \qquad \dots (9a)$$

Similarly from the rules $[\phi(x), \phi(x')] = [\pi(x), \pi(x')] = 0$, we obtain

$$[q_k, q_{k'}] = [p_k, p_{k'}] = 0$$
 ...(9b)

Now we express the Hamiltonian H for the real scalar field in terms of the canonically conjugate variables q_k and p. For it we have,

$$\int \phi^{2}(\mathbf{x}) d^{3}x = \frac{1}{V} \int d^{3}x \sum_{k} \sum_{k'} q_{k} e^{i\mathbf{k} \cdot \mathbf{x}} q_{k'} e^{i\mathbf{k}' \cdot \mathbf{x}}$$

$$= \sum_{k, k'} q_{k}q_{k'} \frac{1}{V} \int d^{3}x e^{i(\mathbf{k} + \mathbf{k}')} \mathbf{x}$$

$$= \sum_{k, k'} q_{k}q_{k'} \delta_{k, -k'}$$

$$= \sum_{k} q_{k}q_{-k} = \sum_{k} q_{k}q_{k} \dagger \{\text{Using eqn. (6)}\}$$

$$= \sum_{k} |q_{k}|^{2} \qquad \dots (10a)$$

Similarly,

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$$\int \pi^{2} (x) d^{3}x = \sum_{k} p_{k} p_{k} \dagger = \sum_{k} |p_{k}|^{2} ... (10b)$$

and

$$\int (\nabla \phi)^2 d^3 x = \frac{1}{V} \int dx^3 \sum_{k, k'} ik \ q_k \ e^{i\mathbf{k} \cdot \mathbf{x}} . ik' . q_{k'} e^{i\mathbf{k}' \cdot \mathbf{x}}$$

$$= \sum_{k, k'} q_k \ q_{k'} (-\mathbf{k} \cdot \mathbf{k}') \ \delta_k, -\mathbf{k}'$$

$$= \sum_{k} \mathbf{k}^2 \ q_k q_k \dagger = \sum_{k} \mathbf{k}^2 |q_k|^2 \qquad \dots (10c)$$

Substituting eqns. (10) into (4) we get the Hamiltonian for the real scalar field as:

$$H = \sum_{k=1}^{\infty} \frac{1}{2} (\omega_k^2 | q_k|^2 + |p_k|^2)$$
; where $\omega_k^2 = (m^2 + k^2)$...(11)

Now the Hamiltonian for a simple harmonic oscillator of unit mass can be written as

$$H = \frac{1}{2} \left(\omega^2 q^2 + p^2 \right) \tag{12}$$

Comparing (11) with (12) we see that the Hamiltonian for the real scalar field is similar to a sum of an infinite number of harmonic oscillators of the ordinary quantum mechanics. Hence the quantization of the field is equivalent to the quantization of these harmonic oscillators

Creation, Annihilation and Nember Operators. Taking analogy from the raising and lowering operators of the simple harmonic oscillator (see matrix theory of harmonic oscillator in section 3·11) we define two operators a_k and a_k † for the description of the field as:

$$a_{k} = \frac{1}{\sqrt{(2\omega_{k})}} \left(\omega_{k} q_{k} + i p_{k} \dagger \right)$$

$$a_{k} \dagger = \frac{1}{\sqrt{(2\omega_{k})}} \left(\omega_{k} q_{k} \dagger - i p_{k} \right)$$

$$\dots (13)$$

It will be seen presently that the description of the quantized field in terms of these operato s can be given a particle interpretation, and using these we can also explain the creation and the destruction of the particles. Moreover, the Hamiltonian for the field will be diagonalized in this representation.

First we develop the algebra of the operators a_k and a_k † from that of the operators q_k and p_k . We have,

$$[a_k, a_k'\dagger] = \frac{1}{2\sqrt{(\omega_k\omega_k')}} \left\{ \omega_k\omega_k' \left[q_k, q_k'\dagger \right] - i\omega_k \left[q_k, p_k' \right] + i\omega_k' \left[p_k\dagger, q_k'\dagger \right] + \left[p_k\dagger, p_k' \right] \right\}$$

$$=\frac{1}{2\sqrt{(\omega_{k}\omega_{k}')}}(2\omega_{k}\delta_{kk}')=\delta_{kk}'$$
...(14a)

$$[a_{i}, a_{i}] = 1$$

Similarly,
$$[a_k, a_{k'}] = a_{k} \dagger, a_{k'} \dagger = 0$$
 ...(14b)

Now we express the Hamiltonian H in terms of the operators a_k and a_k . For this we have from eqn. (13) that

$$q_{k} = \frac{1}{\sqrt{(2\omega_{k})}} (a_{k} + a_{-k} \dagger)$$

$$p_{k} = \sqrt{\left(\frac{\omega_{k}}{2}\right)} i (a_{k} \dagger - a_{-k})$$

$$\dots(15)$$

Substituting these values in equation (11) we get

$$H = \sum_{k} \frac{1}{2} \left(\omega_{k}^{2} \cdot \frac{1}{2\omega_{k}} \left(a_{k} + a_{-k} \dagger \right) \left(a_{k} \dagger + a_{-k} \right) + \frac{\omega_{k}}{2} \left(a_{k} \dagger - a_{-k} \right) \left(a_{k} - a_{-k} \dagger \right) \right)$$

$$= \sum_{k} \frac{1}{2} \left(\frac{\omega_{k}}{2} \left(a_{k} a_{k} \dagger + a_{k} a_{-k} + a_{-k} \dagger a_{k} \dagger + a_{-k} \dagger a_{-k} \dagger a_{-k} \right) \right)$$

$$+\frac{\omega_k}{2}\left(a_k\dagger a_k-a_k\dagger a_{-k}\dagger -a_{-k}a_k+a_{-k}a_{-k}\dagger\right)$$

$$= \sum_{k} \frac{\omega_{k}}{4} \left(a_{k} a_{k} \dagger + a_{-k} a_{-k} \dagger + a_{-k} \dagger a_{k} \dagger - a_{k} \dagger a_{-k} \dagger \right)$$

$$+a_{-1}; +a_{-1}; +a_{1}; +a_{1}; +a_{1}; -a_{-1}; -a_{-1}; a_{1})$$

From (14b) we have $a_{-k}\dagger a_k\dagger - a_k\dagger a_{-k}\dagger = 0$ and $a_ka_{-k} - a_{-k}a_k = 0$. Therefore,

$$H = \sum_{k=0}^{\infty} \frac{\omega_k}{4} \left(a_k a_k \dagger + a_{-k} \dagger + a_{-k} \dagger a_{-k} \dagger a_{-k} \dagger a_{-k} \dagger a_{-k} \dagger a_{-k} \right)$$

Since there is a summation over the index k, we can change it by -k in the second and the third terms without altering the value of the summation, and hence we can write

$$H = \sum_{k} \frac{\omega_{k}}{4} \left(2a_{k}a_{k} \dagger + 2a_{k} \dagger a_{k} \right)$$

$$= \sum_{k} \frac{\omega_{k}}{4} \left(4a_{k} \dagger a_{k} + 2 \right) \qquad \{\text{using } [a_{k}, a_{k} \dagger] = 1\}$$

$$= \sum_{k} \omega_{k} \left(a_{k} \dagger a_{k} + \frac{1}{2} \right)$$

Difining an operator
$$N_k = a_k \dagger a_k$$
, we can write
$$H = \sum_{k} \omega_k \left(N_k + \frac{1}{2} \right) \qquad \dots (16)$$

Using the commutation relations (14), it can be readily seen that the operator N_k satisfies the following relations,

$$[N_k, N_{k'}] = 0 \qquad ...(17a)$$

$$[a_k, N_k] = a_k \qquad ...(17b)$$

$$[a_k \dagger, N_k] = -a_k \dagger \qquad ...(17c)$$

For example,

$$[a_k, N_k] = [a_k, a_k \dagger a_k]$$

$$= [a_k, a_k \dagger] a_k + a_k \dagger [a_k, a_k]$$

$$= 1 \cdot a_k + a_k \dagger \cdot 0$$

$$= a_k.$$

Similarly we can prove the other relations.

We have seen that the operators N_k corresponding to different k values commute. Therefore the observables corresponding to these operators are simultaneously measurable. Thus the operator N_k can be represented by a diagonal matrix. The space in which N_k 's are diagonal is called the Fock Space. Now we find out the eigen-values of operator N_k in a representation in which it is diagonalized and observe the effects of a_k and a_k † on the eigenstates of N_k . The eigenvalue eqn. for N_k can be written as:

$$N_k \mid n_k \rangle = n_k \mid n_k \rangle \qquad ...(18)$$

Using (17b) we have

$$N_k a_k \mid n_k \rangle = (a_k N_k - a_k) \mid n_k \rangle = (n_k - 1) a_k \mid n_k \rangle$$
 ...(19)

Similarly, using (17c) we get

$$N_k a_k \dagger \mid n_k \rangle = (n_k + 1) a_k \dagger \mid n_k \rangle \qquad \dots (20)$$

From (19) and (20) we see that $a_k \mid n_k$ and $a_k \dagger \mid n_k$ are also the eigenstates of operator N_k with eigenvalues (n_k-1) and (n_k+1) ; respectively. Thus we have,

$$a_k \mid n_k \rangle = C_- \mid n_k - 1 \rangle$$
 and $a_k \dagger \mid n_k \rangle = C_+ \mid n_k + 1 \rangle$

where C_{-} and C_{+} are constants and can be found as follows:

$$|C_{+}|^{2} = |C_{+}|^{2} \langle n_{k}+1 | n_{k}+1 \rangle = \langle n_{k} | a_{k}a_{k}\dagger | n_{k} \rangle$$

$$= \langle n_{k} | (a_{k}\dagger a_{k}+1) | n_{k} \rangle$$

$$= \langle n_{k} | (N_{k}+1) | n_{k} \rangle$$

$$= \langle n_{k}+1 \rangle,$$

and

$$|C_{-}|^2 = \langle n_k \mid a_k \uparrow a_k \mid n_k \rangle = n_k$$

Choosing the arbitrary phase factors as unity, we can thus write,

or

or

$$a_{k} \mid n_{k} \rangle = \sqrt{(n_{k}) \mid n_{k} - 1 \rangle}$$

$$a_{k} \uparrow \mid n_{k} \rangle = \sqrt{(n_{k} + 1) \mid n_{k} + 1 \rangle}$$
...(21)

Now we show that the eigenvalues n_k of N_k can take only positive integral values. For it, we can write for the norm of state $a_k \mid n_k$ as:

$$\langle n_k \mid a_k \dagger a_k \mid n_k \rangle \geqslant 0$$

$$\langle n_k \mid N_k \mid n_k \rangle \geqslant 0$$

$$\cdot n_k \geqslant 0$$

The equality sign holds only for the state $|0\rangle$, for which $a_k |0\rangle = 0$. Thus the lowest eigen-value of N_k is zero. Starting from the state $|0\rangle$, we can build up all the higher states by repeated application of the operator $a\dagger$. We have

$$|1\rangle = a_k \dagger |0\rangle$$

$$|2\rangle = a_k \dagger |1\rangle = (a_k \dagger)^2 |0\rangle$$

$$|n\rangle = (a_k \dagger)^n |0\rangle,$$

such that

$$\begin{array}{c|c} N_k & 1 > = 1 & 1 > \\ N_k & 2 > = 2 & 2 > \\ \dots & \dots & \dots \\ N_k & n > = n & n > \end{array}$$

Thus the eigenvalue n_k of N_k takes the values 0, 1, 2, 3, Therefore, the eigenvalue of the Hamiltonian operator H {eqn. (16)} for the field can be written as

$$E = \sum_{k} \omega_{k} (n_{k} + \frac{1}{2}) ; n_{k} = 0, 1, 2, 3, ...$$
 ... (22)

The zero point energy for the field is obtained by putting $n_k=0$ and it is equal to $\frac{1}{2}\sum_k \omega_k$, which is infinite, because k is infinity. Since it is an all k.

infinity Since it is an additive constant, it has got no physical significance. Subtracting this constant from, the Hamiltonian the eqns. of motion are not changed and hence the zero point energy can be subtracted from (22). Thus the energy for the field can be written as:

$$E = \sum_{k} n_{k} \omega_{k} \qquad \dots (23)$$

4

The stationary state of the field has, therefore, the same energy as if there existed n_i number of particles with momentum k and common rest mass m; each particle contributing an "energy quantum" $\omega_k = \sqrt{(m^2 + k^2)}$. Thus the operator N_k can be called a "particle number operator". The operator a_k ; changes the state n_k into $|n_k+1\rangle$; i.e., its operation creates one particle and the

operator a_k changes $|n_k\rangle$ into $|n_{k-1}\rangle$; i.e. its operation destroy one particle. Therefore the operators a_k and a_k ; are named as destruction or annihilation operator and the creation operator; respectively. The operator N_k , on the other hand preserves the number of particles. The operator $N = \sum_k N_k$ is interpreted as

the operator for the total number of particles. Operating on the eigenstate of the field, it yields the total number of particles present in the field. A state in which no particles are present is called the vacuum state. It has no energy and momentum.

We can express the field operators $\phi(x)$ and $\pi(x)$ in terms of the creation and annihilation operators. For it we substitute eqn. (15) into eqn. (5):

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_k)}} \left(a_k e^{i\mathbf{k} \cdot \mathbf{x}} + a_k \dagger e^{-i\mathbf{k} \cdot \mathbf{x}} \right) \dots (24a)$$

$$\tau(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \sqrt{\left(\frac{\omega_k}{2}\right)} i \left(a_k \dagger e^{-i\mathbf{k} \cdot \mathbf{x}} - a_k e^{i\mathbf{k} \cdot \mathbf{x}}\right) \qquad \dots (24b)$$

Using these relations we can very easily find out an expression for the momentum of the field in terms of a_k and a_k ; as:

$$P = \int d^3x \ \pi(\mathbf{x}) \ \nabla \phi \ (\mathbf{x})$$

$$= \sum_{k} \mathbf{k} \ a_k \dagger a_k = \sum_{k} \mathbf{k} \ N_k \qquad \dots (25)$$

13.2. QUANTIZATION OF COMPLEX SCALAR FIELD:

As we have discussed in the last chapter, the complex field describes a charged system. Therefore, in the quantized theory it will describe the charged particles. The quantization of the complex field can be performed in a manner similar to that for the real scalar field. It was first of all carried out by Pauli and Weisskopf.†

The classical complex field is described by the field variables

$$\phi = \frac{\phi_1 + i\phi_2}{\sqrt{(2)}}$$
, and $\phi^* = \frac{\phi_1 - i\phi_2}{\sqrt{(2)}}$;

where ϕ_1 and ϕ_2 are real (see eqn. (38) of last chapter). On the quantum level, ϕ and ϕ^* become non-Hermitian operators

$$\phi = \frac{\phi_1 + i_{12}}{\sqrt{(2)}}$$
; and $\phi \dagger = \frac{\phi_1 - i_{12}}{\sqrt{(2)}}$; $\phi \neq \phi \dagger$.

[†]W. Pauli and V.F. Weisskopf, Helv. Phys, Acta, 7, 709 (1934)

The real sields ϕ_1 and ϕ_2 can be expressed in terms of their creation and annihilation operators as (see eqns. 24)

$$\phi_{1} = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(a_{k}^{(1)} e^{i\mathbf{k} \cdot \mathbf{x}} + a_{k}^{(1)} \dagger e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

$$\phi_{2} = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(a_{k}^{(2)} e^{i\mathbf{k} \cdot \mathbf{x}} + a_{k}^{(2)} \dagger e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

$$\therefore \quad \phi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(\frac{a_{k}^{(1)} + ia_{k}^{(2)}}{\sqrt{(2)}} e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

$$\therefore \quad \phi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(\frac{a_{k}^{(1)} + ia_{k}^{(2)}}{\sqrt{(2)}} e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

$$+\frac{a_k^{(1)}\dagger+ia_k^{(2)}\dagger}{\sqrt{(2)}}e^{-i\mathbf{k}\cdot\mathbf{x}}$$
.

and

$$\phi \dagger (\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(\frac{a_{k}^{(1)} - ia_{k}^{(2)}}{\sqrt{(2)}} e^{i\mathbf{k} \cdot \mathbf{x}} + \frac{a_{k}^{(1)} \dagger - ia_{k}^{(2)} \dagger}{\sqrt{(2)}} e^{-i\mathbf{k} \cdot \mathbf{x}} \right)$$

Introducing the following notations.

$$a_k^{(\pm)} = \frac{a_k^{(1)} \pm ia_k^{(2)}}{\sqrt{(2)}},$$
 ...(27)

we have

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(a_{k}^{(+)} e^{i\mathbf{k} \cdot \mathbf{x}} + a_{k}^{(-)} \dagger e^{-i\mathbf{k} \cdot \mathbf{x}} \right) \dots (28a)$$

and

$$\phi\dagger(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_k)}} \left(a_k^{(-)} e^{i\mathbf{k}\cdot\mathbf{x}} + a_k^{(+)} \dagger e^{-i\mathbf{k}\cdot\mathbf{x}} \right) \dots (28b)$$

The creation and annihilation operators $a_k^{(i)} \dagger$ and $a_k^{(i)}$ for each field ϕ_i (i=1, 2), satisfy commutation rules similar to these of eqn. (14)

$$\begin{bmatrix} a_{k}^{(i)}, a_{k'}^{(i)} \dagger \end{bmatrix} = \delta_{kk'} \delta_{ij} ; i, j = 1, 2
\begin{bmatrix} a_{k}^{(i)}, a_{k'}^{(j)} \end{bmatrix} = \begin{bmatrix} a_{k}^{(i)} \dagger, a_{k'}^{(j)} \dagger \end{bmatrix} = 0
\dots (29)$$

Using these we can find out the commutation rules for ϕ , ϕ † and $a_k^{(+)}$, $a_k^{(-)}$ and their adjoints. We get

$$\left[a_k^{(\pm)}, a_{k'}^{(\pm)\dagger}\right] = \delta_{kk'} \qquad \dots (30)$$

with all other commutators vanishing.

$$[\phi(\mathbf{x}), \phi^{\dagger}(\mathbf{x}')] = i\delta(\mathbf{x} - \mathbf{x}') \qquad \dots (31)$$

Since the operators $a_k^{(\pm)}$ satisfy the commutation rules similar to these for $a_k^{(i)}$ (i=1,2), we can describe the complex field in terms of $a_k^{(\pm)}$ instead of the creation and annihilation operators of the real fields ϕ_1 and ϕ_2 . The operators $a_k^{(\pm)}$ and $a_k^{(\pm)}$; can be interpreted as the destruction and the creation operators for a positively charged field and $a_k^{(-)}$ and $a_k^{(-)}$; are the corresponding operators for a negatively charged field.

Now we express the total Hamiltonian for the complex field in terms of the operators $a_k^{(\pm)}$. For it we have from eqn. (24b) and from the fact that $\pi = \frac{\pi_1 - i\pi_2}{\sqrt{(2)}}$, where π_1 and π_2 are the real momentum densities corresponding to the real fields ϕ_1 and ϕ_2 ,

$$\pi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \sqrt{\left(\frac{\omega_{k}}{2}\right)} i \left(a_{k}^{(+)} \dagger e^{-i\mathbf{k} \cdot \mathbf{x}} - a_{k}^{(-)} e^{i\mathbf{k} \cdot \mathbf{x}}\right) \dots (32a)$$

and, therefore,

$$\pi \dagger (\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \sqrt{\left(\frac{\omega_{k}}{2}\right)} i \left(a_{k}^{(-)} \dagger e^{-ik \cdot \mathbf{x}} - a_{k}^{(+)} e^{ik \cdot \mathbf{x}}\right) \dots (32b)$$

The total Hamiltonian for the quantized complex scalar field can be writen from the Hamiltonian density for the classical field given by eqn. (41) of last chapter, as

 $H = \int d^3x \ H = \int d^3x \ (\pi \dagger \pi + (\nabla \phi \dagger) \ (\nabla \phi) + m^2 \phi \dagger \phi) \quad ...(33)$ Using equations (28) and (32) we have,

$$\int d^3x \, \pi^{\dagger}(\mathbf{x}) \, \pi(\mathbf{x}) = -\frac{1}{V} \sum_{k, \, k'} \frac{\sqrt{(\omega_k \omega_{k'})}}{2} \int d^3x \, \left(a_k^{(+)} \, a_{k'}^{(-)} \, e^{i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}} \right)$$

$$-a_{k}^{(+)} a_{k'}^{(+)} \dagger e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{x}} - a_{k}^{(-)} \dagger a_{k'}^{(-)} e^{-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{x}}$$

$$+a_k^{(-)}+a_{k'}^{(+)}+e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}$$

$$= -\sum_{k,k'} \frac{\sqrt{(\omega_{k'''k'})}}{2} \left(a_{k}^{(+)} a_{k'}^{(-)} \delta_{k}, _{-k'} - a_{k}^{(+)} a_{k'}^{(+)} \dagger \delta_{kk'} - a_{k'}^{(-)} \dagger a_{k'}^{(-)} \delta_{kk'} + a_{k'}^{(-)} \dagger a_{k'}^{(+)} \dagger \delta_{k}, _{-k'} \right)$$

$$= -\sum_{k} \frac{\omega_{k}}{2} \left(a_{k}^{(+)} a_{-k}^{(-)} - a_{k}^{(+)} a_{k}^{(+)} \dagger - a_{k}^{(-)} \dagger a_{k}^{(-)} + a_{k'}^{(-)} \dagger a_{-k}^{(+)} \dagger \right) \dots (34)$$

$$\int \phi \dagger \phi \ d^{3}x = \sum_{k'} \frac{1}{2\omega_{k}} \left(a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(+)} a_{k}^{(+)} \dagger + a_{k'}^{(-)} \dagger a_{k'}^{(-)} + a_{k'}^{(-)} \dagger a_{-k'}^{(+)} \dagger \right)$$
and
$$\dots (35)$$

und

$$\int (\nabla \phi \dagger) (\nabla \phi) d^3x = \sum_{k} \frac{-k^2}{2\omega_k} \left(a_k^{(+)} a_{-k}^{(-)} - a_k^{(+)} a_k^{(+)} \dagger - a_k^{(-)} \dagger a_k^{(-)} + a_k^{(-)} \dagger a_k^{(+)} \dagger - a_k^{(-)} \dagger a_k^{(+)} \dagger - a_k^{(-)} \dagger a_k^{(-)} \right) \dots (36)$$

Substituting (34), (35) and (36) into (33) we get

$$H = \sum_{k} \frac{\omega_{k}}{2} \left[-a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(+)} a_{k}^{(+)} \dagger + a_{k}^{(-)} \dagger a_{k}^{(-)} - a_{k}^{(-)} \dagger a_{-k}^{(+)} \dagger \right]$$

$$+ \sum_{k} \left(\frac{\omega_{k}}{2} - \frac{k^{2}}{2\omega_{k}} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(+)} a_{k}^{(+)} \dagger + a_{k}^{(-)} \dagger a_{k}^{(-)} + a_{k}^{(-)} \dagger a_{-k}^{(+)} \dagger \right]$$

$$+ \sum_{k} \left(\frac{-k^{2}}{2\omega_{k}} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} - a_{k}^{(+)} a_{k}^{(+)} \dagger - a_{k}^{(-)} \dagger a_{k}^{(-)} + a_{k}^{(-)} \dagger a_{-k}^{(+)} \dagger \right]$$

$$+ \sum_{k} \left(\frac{-k^{2}}{2\omega_{k}} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} - a_{k}^{(+)} a_{k}^{(+)} \dagger - a_{k}^{(-)} \dagger a_{k}^{(-)} + a_{k}^{(-)} \dagger a_{-k}^{(+)} \dagger \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right) \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} \right] \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \right] \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \right] \left[a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \right] \left[a_{k}^{(+)} a_{-k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \right] \left[a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \right]$$

$$+ \sum_{k} \left(a_{k}^{(+)} a_{-k}^{(+)} + a_{k}^{(-)} \right] \left[a_{k}^{(+)} a_{-k}^{(+)} \right]$$

or
$$H = \sum_{k} \omega_{k} \left(a_{k}^{(+)} a_{k}^{(+)} \dagger + a_{k}^{(-)} \dagger a_{k}^{(-)} \right)$$

$$+\sum_{k} \left(\frac{-k^{2}}{\omega_{k}}\right) \left(a_{k}^{(+)} a_{-k}^{(-)} + a_{k}^{(-)} \dagger a_{-k}^{(+)} \dagger\right)$$

Using the definitions (27) for $a_k^{(\pm)}$ and the Hermiticity of $a_k^{(i)}$, $a_{-k}^{(i)}$ (i=1, 2), it can very easily be seen after a little algebra that the second term on the r.h.s. of the above equation vanishes.

$$H = \sum_{k} \omega_{k} \left(a_{k}^{(+)} a_{k}^{(+)} \dagger + a_{k}^{(-)} \dagger a_{k}^{(-)} \right)$$

$$= \sum_{k} \omega_{k} \left(a_{k}^{(+)} \dagger a_{k}^{(+)} + a_{k}^{(-)} \dagger a_{k}^{(-)} + 1 \right) \qquad ...(37)$$
[Using eqn. (30)]

Defining the particle number operators $N_k^{(+)} = a_k^{(+)} \dagger a_k^{(+)}$ and $N_k^{(-)} = a_k^{(-)} \dagger a_k^{(-)}$ for the positively and the negatively charged particles; respectively, we can write:

$$H = \sum_{k} \omega_{k} \left(N_{k}^{(+)} + N_{k}^{(-)} + 1 \right) \qquad \dots (38)$$

It is left as an exercise for the readers to show that the momentum,*

$$\mathbf{P} = -\int d^3x [\pi(\mathbf{x}) \nabla \phi(\mathbf{x}) + \pi \dagger(\mathbf{x}) \phi \dagger(\mathbf{x})].$$

for the complex field can be expressed as:

$$P = \sum_{k} k \left(N_{k}^{(+)} + N_{k}^{(-)} \right) \qquad ...(39)$$

Now we derive an expression for the total charge of the field in terms of the number operators $N_k^{(+)}$ and $N_k^{(-)}$. The total charge operator for the complex scalar field is defined by (classical charge density is given by equation (46-b) of last chapter)

$$Q = i\epsilon \int d^3x (\dot{\phi}\dot{\phi}\dagger - \dot{\phi}\dagger \dot{\phi})\dagger \equiv i\epsilon \int d^3x (\pi\dagger \dot{\phi}\dagger - \pi \dot{\phi})$$

Using eqns. (28) and (32) in it we can easily show that

$$Q = \epsilon \sum_{k} \left(a_{k}^{(+)} \dagger a_{k}^{(+)} - a_{k}^{(-)} \right)$$

^{*}Classical momentum density for the complex scalar field can be obtained by using the eqns. (i) and (vi) of prob. 1 of last chapter. Lagrangian density L in (i) we have to use expression (39) of last chapter.

$$=\epsilon \sum_{k} \left(N_{k}^{(+)} - N_{k}^{(-)} \right) \qquad \dots (40)$$

Thus the positive and the negative quanta carry $+\epsilon$ and $-\epsilon$ units of charges, respectively.

We can now say that $a_k^{(+)}$, $a_k^{(+)}$; and $N_k^{(+)}$ are annihilation, creation and particle number operators for a scalar particles of energy a_k momentum k and electric charge $+\epsilon$. The operators $a_k^{(-)}$, $a_k^{(-)}$; and $N_k^{(-)}$ are the corresponding operators for particles of charge $-\epsilon$. We can identify the quanta with positive charges as the particles and those with negative charges as their antiparticles.

The Hamiltonian, the momentum and the total charge operators are all expressed in terms of $N_k^{(+)}$ and $k^{(-)}$ and hence these are all diagonal

13.3. QUANTIZATION OF SCHRODINGER'S FIELD:

The non-relativistic Schrodinger's field can be quantized by treating the field variables $\psi(x)$ and $\pi(x)$ as operators satisfying the commutation rules (2). The Hamiltonian density for a classical Schroedinger field is given by (eqn. (50) of last chapter)

$$\mathbf{H} = \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi + V \psi^* \psi$$

Hence the total Hamiltonian for a quantized field cax be written as:

$$H = \int d^3x \left(\frac{\hbar^2}{2m} \nabla \psi \dagger \cdot \nabla \psi + V \psi \dagger \psi \right) \qquad \dots (41)$$

It is a Hermitian operator.

In order to find the consequences of the quantization of the field, we expand the field variable $\psi(x)$ in terms of the complete set of orthonormal eigenfunctions ' u_k (x)' of the quantum meahanical

Hamiltonian,
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)$$
,

$$\psi(\mathbf{x}) = \sum_{k} a_k u_k(\mathbf{x}),$$

$$\psi(\mathbf{x}) = \sum_{k} a_k u_k(\mathbf{x}),$$

$$\dots(42)$$

where
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)u_k(\mathbf{x}) = E_k u_k(\mathbf{x})$$
For the quantized field, $I(\mathbf{x})$:

For the quantized field, $\psi(x)$ is an operator, and hence coefficients a_k are operators and serve as the dynamical variables of

01.

the field, while $u_k(x)$ are just algebric functions. Thus from (42) we have

 $\psi \dagger(\mathbf{x}) = \sum_{k} a_k \dagger u_k^*(\mathbf{x}) \qquad \dots (43)$

The operators a_k and a_k ; are the destruction and creation operators for the Schroedinge's field and we can derive their commutators from that for the field operators $\psi(x)$ and ψ ; (x). We have,

 $[\psi(\mathbf{x}), \pi(\mathbf{x}')] = i \hbar \delta^3(\mathbf{x} - \mathbf{x}')$ $[\psi(\mathbf{x}), i \hbar \psi \dagger (\mathbf{x}')] = i \hbar \delta^3(\mathbf{x} - \mathbf{x}')$ $\vdots [\psi(\mathbf{x}), \psi \dagger (\mathbf{x}')] = \delta^3(\mathbf{x} - \mathbf{x}')$

{:: classical momentum density is given by $\pi(x) = i\hbar \psi^*$; see section 12.7}

Using this relation, we can find the value of the commutator $[a_k, a_k'\dagger]$. For it, we muitiply (42) by u_k^* (x) and (43) by u_k and integrate over the entire space. We get

grate over the entire epoch
$$a_k = \int d^3x \, u_k(\mathbf{x}) \psi(\mathbf{x})$$
 and $a_k \dagger = \int d^3x \, u_k(\mathbf{x}) \psi^{\dagger}(\mathbf{x})$.

$$[a_k, a_k' \dagger] = \int d^3x \int d^3x' \, [\psi(\mathbf{x}), \psi^{\dagger}(\mathbf{x}')] \, u_k^*(\mathbf{x}) \, u'_k(\mathbf{x}')$$

$$= \int d^3x \int d^3x' \, \delta^3(\mathbf{x} + \mathbf{x}') \, u_k^*(\mathbf{x}) \, u_k'(\mathbf{x}')$$

$$= \int d^3x \, u_k^*(\mathbf{x}) \, u_k'(\mathbf{x}) = \delta_{kk'} \qquad ...(44)$$

Similarly it can be shown that all the other commutators of of a_k and a_k † vanish.

Now we express the total Hamiltonian H in terms of a_k and a_k . For it we substitute (42) and (43) into (41). We get;

$$H = \sum_{k, k'} a_k i a_{k'} \left[\frac{\hbar^2}{2m} \int d^3x \, \nabla u_k^*(\mathbf{x}) . \, \nabla u_{k'}(\mathbf{x}) \right]$$

 $+ \int d^3x V \, u_k^*(\mathbf{x}) \, u_k'(\mathbf{x}) \, \bigg]$

Evaluating the first integral by parts and noting that the second part vanishes for the infinite surface of integration, we can write the above equation as:

$$H = \sum_{k, k'} a_k \dagger a_{k'} \left[-\frac{\hbar^2}{2m} \int u_k^*(\mathbf{x}) \nabla^2 u_{k'}(\mathbf{x}) d^3 x + \int V u_k^*(\mathbf{x}) u_{k'}(\mathbf{x}) d^2 x \right]$$

$$= \sum_{k, k'} a_k \dagger a_{k'} \int u^*_k(\mathbf{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] u_{k'}(\mathbf{x}) d^3 x.$$

$$= \sum_{k, k'} a_k \dagger a_{k'} \int u_k^*(\mathbf{x}) E_{k'} u_{k'}(\mathbf{x}) d^3 x.$$

$$= \sum_{k,k'} a_k \dot{a}_k' E'_k \delta_{kk'} = \sum_k a_k \dot{a}_k E_k$$

Defining the number operator $N_k = a_k \dagger a_k$, we have,

$$H = \sum_{k} N_{k} E_{k}$$
...(45)

It can easily be shown that the number operators corresponding to different values of k commute with each other. Hence we can diagonalize all the N_k 's simultaneously. In the diagonal representation, N_k has eigenvalues as zero and positive integers and no other values. When N_k is diagonal, then we see from (45) that the Hamiltonian will also be diagonal.

13.4. QUANTIZATION OF DIRAC'S FIELD:

Before quantizing the Dirac field we discuss about the difficulties of the relativistic unquantized Dirac wave equation.

First of all, the Dirac wavefunction of the unquantized theory describes only a single particle and hence it is not possible to describe in terms of it the phenomena like pair production and pair annihilation.

Though we described the phenomena like pair production and pair annihilation, but instead of using the language that the number of electrons is not conserved, we said that the number of electrons is actually conserved and that happens is just the escalation of a negative-energy electron. Thus we tried to explain the phenomena liwe pair production with the single particle interpretation of the Dirac wavefunction. In doing so, however, we had to depart very radically from the single particle theory itself; because we had to introduce the concept of Dirac sea, an infinite number of negative energy electrons.

The success of the hole theory lies in the fact that the electrons satisfy the Pauli's Exclusion principle and although electrons and positrons can be created or annihilated, the interaction in electro-dynamics is such that the difference between the number of electrons and the number of positrons

$$N = N(e^{-}) - N(e^{+})$$

However, in the Nature, there are nonelectromagnetic phenois conserved. mena which do not conserve N; e. g., in β -decay

$$p\rightarrow n+e^{+}+v$$

according to hole theory, the presence of the e+ in the final state should be due to the absence of a negative energy electron in the Dirac sea. But where is the electron; which used to occupy the new vacated negative energy state. It seems that the probability of finding the electrons is no longer conserved. In order to resolve the above difficulties, we have to quantize the Dirac field. We try to carry out the quantization of the Dirac field in a manner similar to that for the Schrodinger's field; though at this stage we do not know exactly whether this method is a legitmate one.

We expand the field variables $\psi(x)$ in terms of the complete set of normalized plane wave solutions of the Dirac equation for positive and negative energies as (see eqn. (ii) of prob. 4, chap-

ter-10).

$$\psi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} \left[b_{rp}(t) u^r(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}} + b'_{rp}(t) v^r(\mathbf{p}) e^{-i\mathbf{p} \cdot \mathbf{x}} \right] \dots (46)$$

In the above expression b_{rp} and b'_{rp} are the coefficients of expansion; $u^r(p)$ and $v^r(p)$ are the positive and the negative energy spinors; respectively, and they satisfy the Dirac equations (see eqns. (73), chapter-10)

 $(-i\overset{\rightarrow}{\alpha} \cdot \nabla + m\beta) u^{r} (\mathbf{p}) = E_{p}u^{r} (\mathbf{p})$ $(-i\overset{\rightarrow}{\alpha} \cdot \nabla + m\beta) v^{r} (\mathbf{p}) = -E_{p}v^{r} (\mathbf{p})$...(47)

and

The Dirac's spinors satisfy the following orthogonality and normalization relations (see section 10.5)

For the quantized field, where $\psi(\mathbf{x})$ is treated as operator, the coefficients b_{rp} and b'_{rp} behave like operators and serve as the dynamical variables, of the field; while $u^r(\mathbf{p})$ and $v^r(\mathbf{p})$ are just algebraic functions. Thus we can write from (46) that

$$\psi^{\dagger}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{x}} \int \left(\frac{m}{E_p} \right) \left[b_{rp}^{\dagger}(t) \cdot u^{r\dagger}(\mathbf{p}) \text{ exp. } (-i\mathbf{p} \cdot \mathbf{x}) + b_{rp}^{\prime\dagger}(t) v^{r\dagger}(\mathbf{p}) \text{ exp. } (i\mathbf{p} \cdot \mathbf{x}) \right] \qquad \dots (49)$$

The operators b_{rp} , b'_{rp} b^{\dagger}_{rp} and b'^{\dagger}_{rp} are the destruction and the creation operators for the Dirac field, and we shall explain their significance, shortly. First we express the total Hamiltonian for the field in terms of these operators. The classical expression

for the total Hamiltonian of the Dirac field has been derived in the last chapter (eqn. (56)) as:

$$H = \int \psi^{\dagger} \left(-i \alpha \cdot \nabla + m\beta \right) \psi d^3x.$$

In order to get the Hamiltonian operator for the quantized field, we substitute eqns. (46) and (49) into it. We obtain

$$H = \frac{1}{V} \int d^3x \sum_{r, p} \sum_{r, p'} \sqrt{(E_p E_{p'})} \left[b_{rp}^{\dagger} u'^{\dagger}(\mathbf{p}) \exp. (-i\mathbf{p}.\mathbf{x}) + b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x}) \right]$$

$$+ b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x})$$

$$+ \left[b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x}) + b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (-i\mathbf{p}.\mathbf{x}) \right]$$

$$= \frac{1}{V} \int d^3x \sum_{r, p} \sum_{r', p'} \frac{m}{\sqrt{(E_p E_{p'})}} \cdot E_{p'} \left[b_{rp}^{\dagger} u'^{\dagger}(\mathbf{p}) \exp. (-i\mathbf{p}.\mathbf{x}) + b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x}) \right] \cdot \left[b_{r'p'} u^{r'}(\mathbf{p}') \exp. (i\mathbf{p}.\mathbf{x}) - b_{r'p'}^{\dagger} v^{r'}(\mathbf{p}') \exp. (-i\mathbf{p}'.\mathbf{x}) \right]$$

$$+ b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x}) \cdot \left[b_{r'p'} u^{r'}(\mathbf{p}') \exp. (-i\mathbf{p}'.\mathbf{x}) \right]$$

$$+ b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x}) \cdot \left[b_{r'p'} u^{r'}(\mathbf{p}') \exp. (-i\mathbf{p}'.\mathbf{x}) \right]$$

$$+ b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (47)$$

$$+ b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (i\mathbf{p}.\mathbf{x}) \cdot \left[b_{r'p'} u^{r'}(\mathbf{p}') \exp. (-i\mathbf{p}'.\mathbf{x}) \right]$$

$$+ b_{rp}^{\dagger} v^{r\dagger}(\mathbf{p}) \exp. (47)$$

Using the relations (48) and

$$\frac{1}{V}\int d^3x \exp \left[\pm i\left(\mathbf{p}-\mathbf{p'}\right).\mathbf{x}\right] = \delta_{pp'},$$

we can write the Hamiltonian as

$$H = \sum_{r,p} \sum_{r',p'} \frac{mE_{r'}}{\sqrt{(E_{p}E_{p'})}} \left[b_{rp}^{\dagger} b_{r'p'} u^{r\dagger}(\mathbf{p}) u^{r'}(\mathbf{p}') \delta_{pp'} \right]$$

$$-b_{rp}^{\prime\dagger} b_{r'p'}^{\prime} v^{r\dagger}(\mathbf{p}) v^{r'}(\mathbf{p}') \delta_{pp'}$$

$$= \sum_{r,p} \sum_{r'} \frac{mE_{p}}{E_{p}} \left[b_{rp}^{\dagger} b_{r'p} u^{r\dagger}(\mathbf{p}) u^{r'}(\mathbf{p}) \right]$$

$$-b_{rp}^{\prime\dagger} b_{r'p}^{\prime\dagger} v^{r\dagger}(\mathbf{p}) v^{r'}(\mathbf{p})$$

$$-b_{rp}^{\prime\dagger} b_{r'p}^{\prime\dagger} v^{r\dagger}(\mathbf{p}) v^{r'}(\mathbf{p}) \right]$$

$$= \sum_{r,p} \sum_{r'} m \left(b_{rp}^{\dagger} b_{r'p} \frac{E_{p}}{m} \delta_{rr'} - b_{rp}^{\prime\dagger} b_{r'p}^{\prime} \frac{E_{p}}{m} \delta_{rr'} \right)$$

$$= \sum_{r,p} E_{p} \left(b_{rp}^{\dagger} b_{rp} - b_{rp}^{\prime\dagger} b_{rp}^{\prime} \right) \dots (50)$$

Now we see that the quantization of Dirac field in a manner similar to that for the Schroedinger's field posses two problems:

Firstly, if we interpret $b^{\dagger}b$ and $b^{\prime}b'$ as the number operators, respectively for the positive and negative energy particles, the total Hamiltonian (50) can be negative also, since E_p can negative. The negative Hamiltonian makes no physical sense, because the energy should be positive definite.

Secondly, the Dirac particles should obey the Pauli's Exclusion principle. However, the quantization using the commutators lead to the Bose-Einstein's statistics.

The second difficulty was resolved by Jordan and Wigner*. They developed a quantization scheme which is equivalent to the Pauli principle (i.e. antisymmetric functions). In this scheme the operators, instead of satisfying commutation rules, satisfy "anticommutation" rules; i.e.,

$$\begin{bmatrix} \psi(\mathbf{x}), \psi^{\dagger}(\mathbf{x}') \end{bmatrix}_{+} = \psi(\mathbf{x}) \psi^{\dagger}(\mathbf{x}') + \psi^{\dagger}(\mathbf{x}') \psi(\mathbf{x}) = \delta^{3} (\mathbf{x} - \mathbf{x}') \\ [\psi(\mathbf{x}), \psi(\mathbf{x}')]_{+} = [\psi^{\dagger}(\mathbf{x}), \psi^{\dagger}(\mathbf{x}')]_{+} = 0 \end{bmatrix} \dots (5)$$

Using these, we can also find the anticommutators for the creation and the annihilation operators. Multiplying (6) by

$$\frac{1}{\sqrt{(V)}}u^{r\dagger}(\mathbf{p})\exp.\left(-i\mathbf{p}.\mathbf{x}\right)$$

and integrating over the space, we obtain:

$$b_{r\nu}(t) = \frac{1}{\sqrt{(V)}} \cdot \sqrt{\binom{m}{E_p}} \int d^3x \, \psi(\mathbf{x}) \, u^{r\dagger}(\mathbf{p}) \, \exp. \, (-i\mathbf{p} \cdot \mathbf{x}),$$

Similarly from (49), we have,

$$b_{rp}^{\dagger}(i) = \frac{1}{\sqrt{(V)}} \sqrt{\left(\frac{m}{E_p}\right)} \int d^3x \ \psi^{\dagger}(\mathbf{x}) \ u^r \ (\mathbf{p}) \ \exp. \ (i\mathbf{p.x})$$

Hence the equal time anticommutator,

$$\begin{bmatrix} b_{rp}, b_{r'p'}^{\dagger} \end{bmatrix}_{+} = \frac{1}{V} \frac{m}{E_{p}} \int d^{3}x \int d^{3}x' \left[\psi(\mathbf{x}), \psi^{\dagger}(\mathbf{x}'), \right]_{+} u^{r\dagger}(\mathbf{p}) u^{r'}(\mathbf{p}') \\ \times \exp\left[(-i\mathbf{p}.\mathbf{x} + i\mathbf{p}'.\mathbf{x}') \right] \\ = \frac{1}{V} \frac{m}{E_{p}} \int d^{3}x u^{r\dagger}(\mathbf{p}) u^{r'}(\mathbf{p}') \exp\left[(-i(\mathbf{p} - \mathbf{p}').\mathbf{x}) \right] \\ \left\{ \vdots, \left[\psi(\mathbf{x}), \psi^{\dagger}(\mathbf{x}') \right]_{+} = \delta^{3} (\mathbf{x} - \mathbf{x}') \right\} \\ \left[b_{r\nu}, b_{r'p'}^{\dagger} \right]_{+} = \frac{m}{E_{p}} u^{r\dagger}(\mathbf{p}) u^{r'}(\mathbf{p}') \delta_{,p'} \end{bmatrix}$$

^{*}P. Jordan and E. P. Wigner, Zeits. für Phys., 47, 631 (1928).

$$= \frac{m}{E_p} \cdot \frac{E_p}{m} \cdot \delta_{rr'} \delta_{pp'}$$

$$= \delta_{rr'} \delta_{pp'} \qquad ...(52a)$$

Similarly,

$$\left[b'_{rp},b'_{r'p'}^{\dagger}\right]_{+}=\delta_{rr'}\delta_{pp'} \qquad ...(52b)$$

In order to see the consequence of the anticommutation rules, we define the number operators for the positive and the negative energy particles; respectively, as

$$N_{rp} = b_{rp}^{\dagger} b_{rp}$$
 and $N'_{rp} = b'_{rp}^{\dagger} b'_{rp}$...(53)

Then,

$$N_{rp}^{2} = b_{rp}^{\dagger} b_{rp} b_{rp}^{\dagger} b_{rp} = b_{rp}^{\dagger} \left(1 - b_{rp}^{\dagger} b_{rp}\right) b_{rp} \qquad \text{(Using 52a)}$$

$$= b_{rp}^{\dagger} b_{rp} - b_{rp}^{\dagger} b_{rp}^{\dagger} b_{rp}^{\dagger} b_{rp} b_{rp}$$

Using (51) we can also show that

$$[b_{rp}, b_{r'p'}]_{+} = [b_{rp}^{\dagger}, b_{r'p'}^{\dagger}]_{+} = 0$$

$$\therefore b_{rp} b_{rp} = b_{rp}^{\dagger} b_{rp}^{\dagger} = 0$$

and hence, we have

$$N_{rp}^2 = b_{rp}^{\dagger} b_{rp} = N_{rp}$$

or

$$N_{rp}(N_{rp}-1)=0 \Rightarrow N_{rp}=0 \text{ or } 1.$$

Thus the possible occupation number for the state of the Dirac field can be zero or one, in accordance with the Pauli's principle.

The first difficulty was removed by Dirac himself. He defined the vacuum state as that state in which all the negative energy states are occupied, i.e. $N'_{rp}=1$, and all the positive energy states are empty, i.e. $N_{rp}=0$. Now the total energy of the Dirac field is given by the Hamiltonian,

$$H = \sum_{r, p} E_{p} \left(b_{rp}^{\dagger} b_{rp} - b_{rp}^{\dagger} b_{rp}^{\dagger} b_{rp}^{\dagger} \right) = \sum_{r, p} E_{p} \left(N_{rp} - N_{rp}^{\prime} \right)$$

Hence the energy of the vacuum state is given by

$$H_{vac} = -\sum_{r,p} E_p (1)_{rp}$$

It is an infinite quantity and for it Dirac gave the hypothesis that it is an unobservable. Only the difference between H and H_{vac} , is the observable value of the energy. Therefore,

$$H_{obs} = H - H_{vac} = \sum_{r, p} E_p \{ N_{rp} + (1 - N'_{rp}) \}. \qquad ...(54)$$

Since, N'rp can take only the values zero and one, the obser-

vable energy of the field is always positive.

Now we derive an expression for the charge operator for the Dirac field in terms of the number operators N_{rp} and N'_{rp} . The classical expansion for the total charge of the Dirac field is given by

$$Q = e \int \psi^{\dagger} \psi d^3x.$$

Using (46) and (49) into it we get the charge operator for the field as

$$Q = e \sum_{r, p} \left(b_{rp}^{\dagger} b_{rp} + b'_{rp}^{\dagger} b'_{rp} \right) = e \sum_{r, p} (N_{rp} + N'_{rp}) \qquad ...(55)$$

$$\therefore Q_{vac} = e^{\sum_{i=1}^{n} (1)_{rp}}$$

It is an infinite quantity and hence it is not an observable. According to Dirac's hypothesis the observable charge is given by

$$Q_{obs} = Q - Q_{vac} = e \sum_{r, p} \{N_{rp} - (1 - N'_{rp})\} \qquad ...(56)$$

It is clear that the observable value of the total charge of

the Dirac field may be positive as well as negative.

Equations (54) and (56) are the mathematical statements for Dirac's hole theory. These eqns. shows that the negative energy states contribute to the total energy and the total charge only when these are unoccupied, i.e. $N'_{rp}=0$. The contribution to the charge from an empty negative emergy state is of opposite sign (-e) than that of the positive energy state. On the other hand, the contribution to the energy from an unoccupied negative energy state as well as from an occupied positive energy state is positive (+ E_p). Thus the absence of a particle in negative energy state corresponds to the presence of a positive energy particle of opposite charge, called the "positron" in the case of electrons, while in general it is called an "antiparticle". Thus the operator $N''_{rp}=(1-N'_{rp})$ can

be referred to as the occupation number for the antiparticle. N''_{rp} can have only the values zero and one.

So far we have given a negative aspect of the antiparticles. We can also give a positive definition for the antiparticle by redefining the operators for the negative energy states as

$$b'_{rp} = d_{rp}^{\dagger} \text{ and } b'_{rp}^{\dagger} = d_{rp}.$$

$$\vdots \left[b'_{rp}, b'_{r'p'}^{\dagger} \right]_{+} = \delta_{pp'} \delta_{rr'} \Rightarrow$$

$$\left[d_{rp}^{\dagger}, d_{r'p'}^{\dagger} \right]_{+} = \delta_{pp'} \delta_{rr'} \qquad \dots (57)$$

$$\vdots d_{rp}^{\dagger} d_{rp} = \left(1 - d_{rp} d_{rp}^{\dagger} \right) = \left(1 - b'_{rp}^{\dagger} b'_{rp} \right) = (1 - N'_{rp}) = N''_{rp}$$

Thus, $d_{rp}^{\dagger} d_{rp}$ is the occupation number for the antiparticle. The operators d_{rd}^{\dagger} and d_{rp} are now the creation and annihilation operators for the antiparticles. The field operator ψ (x) and ψ^{\dagger} (x) can now be written in terms of the creation and annihilation

operators for the antiparticles as: $\psi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{r} \sqrt{\binom{m}{E_p}} [b_{rp}(t) u^r(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}} + d_{rp}^{\dagger}(t) v^r(\mathbf{p})$

$$\times e^{-i\mathbf{p}.\mathbf{x}}$$
] ...(58a)

$$\psi^{\dagger}(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} \left[b_{rp}^{\dagger}(t) u_r^{\dagger}(\mathbf{p}) e^{-i\mathbf{p}.\mathbf{x}} -d_{rp}(t) v^{r\dagger}(\mathbf{p}) e^{i\mathbf{p}.\mathbf{x}}\right] \dots (58b)$$

It is seen that $\psi(x)$ involves the creation of an antiparticle and the destruction of a particle, while $\psi^{\dagger}(x)$ involves the creation of a particle and the destruction of an antiparticle.

13.5. QUANZITATION OF MAXWELL'S FIELD:

Maxwell's Radiation field is a real vector field with zero mass. It is described by the field variables $A_{\mu} = (A, i\phi)$, where A and ϕ are respectively the vector and the scalar potentials. It can also be described equivalently in terms of electric and the magnetic field strength vectors E and B.

For the quantized Radiation field, A, and \u03c4, becomes operators satisfying the commutation rules of the form (3). Now, the component π_4 of the momentum vanishes identically, therefore, A_4 will commute with all the other components of the field operators and hence it will just be a scalar and not an operator, in contrast to the space components A_i (x, t). Thus the quantization procedure is not manifestly covariant. Gupta and Bleuler† gave a covariant procedure for the quantization of the e.m. field; but it abandons the notion, we have cherished so far, of a positive definite norm. We donot go for this method and follow only the historical procedure of canonical quantization with the conviction that our starting point, Maxwell's equations are Lorentz covariant, and though we shall encounter along the way many expressions which are neither Lorentz nor Gauge invariant, the results at the end are Lorentz invariant and are independent of the Gauge. For the equal time commutators of $\pi_t(x, t)$ and $A_i(x, t)$ we are led by the canonical procedure to write

$$[A_{i}(\mathbf{x}, t), A_{j}(\mathbf{x}', t] = [\pi_{i}(\mathbf{x}, t), \pi_{j}(\mathbf{x}', t)] = 0 \qquad ...(59a)$$

$$[A_{i}(\mathbf{x}, t), \pi_{j}(\mathbf{x}', t)] = i\delta_{ij}\delta^{3}(\mathbf{x} - \mathbf{x}') \qquad ...(59b)$$
Since $\tau_{j}(\mathbf{x}', t) = -E_{j}(\mathbf{x}', t)$, we can also write (59b) as
$$[A_{i}(\mathbf{x}, t), -E_{j}(\mathbf{x}', t)] = i\delta_{ij}\delta^{3}(\mathbf{x} - \mathbf{x}') \qquad ...(59c)$$

Now, from the Maxwell's equations we have $\triangle x' \cdot \mathbf{E}(x' t) = 0$

i.e.
$$\sum_{j=1}^{3} \frac{\partial E_{j}(\mathbf{x}'.t)}{\partial x'_{j}} = 0.$$

Therefore, divergence of the left hand side of (59c) vanishes. For consistency, the divergence of the r.h.s should also vanish. However, the divergence of the r.h.s. is not zero. To be out of this screwing difficulty, we should either change the commutation relation or we should modify the equation of motion. But the equations of motion are the experimentally verified results and cannot be changed. So we modify the commutation relation. The δ -function on the r h.s of (59b) is defined by

$$\delta_{ij} \delta^{3}(\mathbf{x} - \mathbf{x}') = \frac{1}{(2\pi)^{3}} \int \delta_{ij} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} d^{3}k$$

We modify it to a divergence less δ -function, called the transverse δ -function, defined as:

[†] S.N. Gupta, Proc. Phys. Soc. (London). A63, 681 (1958) K. Bleuler, Helv. Phys Acta, 3, 567 (1950)

$$\delta_{ij}^{tr.}(\mathbf{x}-\mathbf{x}') = \frac{1}{(2\pi)^3} \int \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right) e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')} d^3k \qquad ...(60)$$

The divergence of it is seen to be zero as:

$$\sum_{j=1}^{3} \frac{\partial}{\partial x'_{j}} \delta_{ij}^{tr.} (x-x') = \sum_{j=1}^{3} \frac{1}{(2\pi)^{3}} \int (-i) \left(k_{i} - \frac{k_{i}k_{j}k_{j}}{k^{2}}\right) e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')} d^{3}k$$

$$= 0.$$

Thus we modify the commutator (59b) to the relation:

$$[A_i(\mathbf{x}, t), \pi_j(\mathbf{x}', t)] = i\delta_{ij}^{tr}(\mathbf{x} - \mathbf{x}')$$
 ...(61)

It should be noticed that the condition,

$$\sum_{i} \frac{\partial}{\partial x_{i}} [A_{i}(\mathbf{x}, t), \pi_{j}(\mathbf{x}, t)] = 0,$$

requires $\frac{\partial A_i}{\partial x_i} = 0$ or $\triangle .A = 0$. It is known as the transversability condition and the vector field satisfying this condition is termed as "transverse field" or "radiation field". For such fields we deal only with the transverse components and forget about the two longitudinal components. We can write A in terms of the transverse and the longitudinal components as:

$$A = A_{trans} + A_{10ng}$$
.

Then $\nabla .A_{trans} = 0$ and $\nabla \times A_{10ng} = 0$; i.e., only the transverse components satisfy the transversability condition. Thus for the radiation field we have to deal with only two transverse degrees of freedom of the sield, but it is at the cost of the Lorentz covariance.

Taking analogy from the real scalar field eqn. (24a), here for the real vector field A(x, t), we can write in the momentum

A
$$(x, t) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega k)}} \sum_{\lambda=1, 2} \hat{\epsilon}_{k, \lambda} \left[a_{k, \lambda}(t) e^{ik.x} + a_{k, \lambda}^{\dagger}(t) e^{-ik.x} \right], \dots (62)$$

ere $\hat{\epsilon}_{k, \lambda}(\lambda=1, 2)$ are the unit polarization.

where $\hat{\epsilon}_{k,\lambda}(\lambda=1,2)$ are the unit polarization vector and $\hat{\epsilon}_{k,1}(\lambda=1,2)$ and $k = \frac{k}{|k|}$ form a set of orthogonal vectors as shown in the fig.

(1). From the orthogonality of ϵ_k , 1, ϵ_k , 2 and ϵ_k we have:

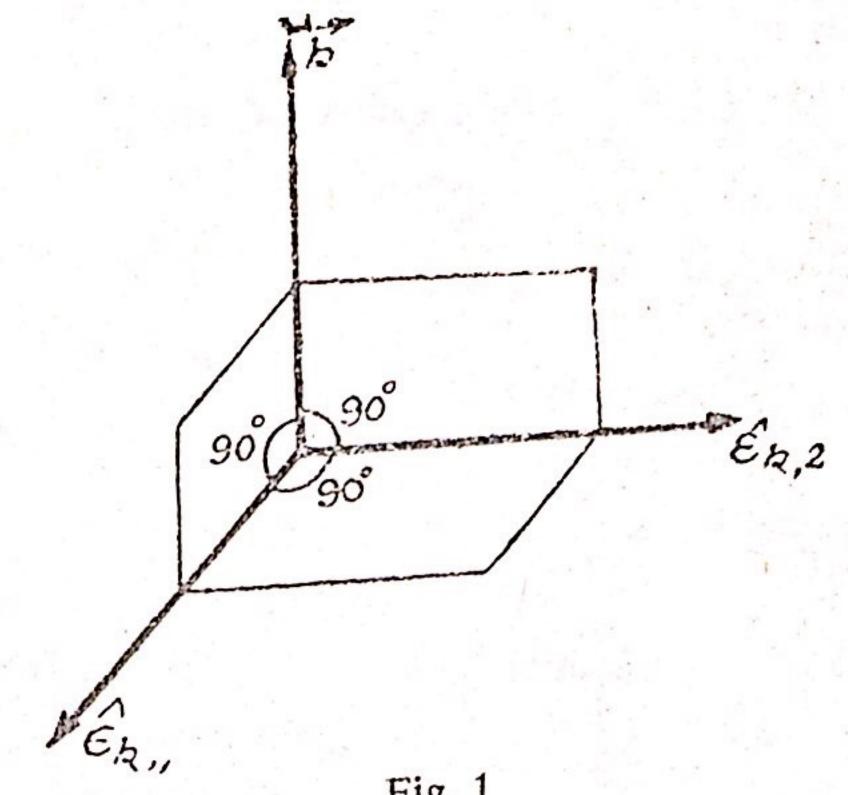


Fig. 1 $\hat{\epsilon}_{k,\lambda}\hat{\epsilon}_{k,\lambda'} = \sum_{i=1}^{\epsilon} (\hat{\epsilon}_{k,\lambda})_i (\hat{\epsilon}_{k,\lambda'})_i = \delta_{\lambda\lambda'}$ $\sum_{i=1}^{n} (\hat{\epsilon}_{k,\lambda})_{i} (\hat{\epsilon}_{k,\lambda})_{j} = \delta_{ij} - \frac{k_{i}k_{j}}{k^{2}}$

and

For further discussion it will be convenient to write the time dependence of a_k , λ (1) explicitly. We have

$$a_{k,\lambda}^{(t)}(t) = a_{k,\lambda}^{(0)}(0) e^{-i\omega_k t}$$

Therefore,

Therefore,
$$A(\mathbf{x},t) = \frac{1}{\sqrt{(V)}} \sum_{k,\lambda} \frac{\hat{\epsilon}_{k},\lambda}{\sqrt{(2\omega_{k})}} \left(a_{k},\lambda^{(0)} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_{k}t} + a_{k}^{\dagger},\lambda^{(0)} e^{-i\mathbf{k}\cdot\mathbf{x} + i\omega_{k}t} \right) \dots (64)$$

From our previous experience, we call a_k , λ and a_k^{\dagger} , as the photon annihilation and creation operators and define the following commutation rules for them.

$$\begin{bmatrix} a_{k}, \lambda, a_{k'}^{\dagger}, \lambda' \end{bmatrix} = \delta_{kk'} \delta_{\lambda \lambda'}, \qquad (65)$$

with all the other commutators between a_k , λ and a_k^{\dagger} , λ as vanish

We can, at once, verity that the commutation rules (59) ing. follows from (65). For example.

$$[A_{i}(\mathbf{x},t), \pi_{j}(\mathbf{x}',t)] = \begin{bmatrix} A_{i}(\mathbf{x},t), \frac{\partial A_{j}(\mathbf{x}',t)}{\partial t} \end{bmatrix}$$

$$\left\{ \pi_{j} = \frac{\partial A_{j}}{\partial t} + \frac{\partial \phi}{\partial x_{j}} \text{ and } \phi = 0 \text{ for the "radiation field"} \right\}$$

$$= \frac{1}{V} \sum_{k,\lambda} \sum_{k',\lambda'} \frac{\left(\hat{\epsilon}_{k,\lambda}\right)_{i} \left(\hat{\epsilon}_{k',\lambda'}\right)_{j}}{2\sqrt{(\alpha_{k}\omega_{k'})}} . i\omega_{k'} \left\{ \begin{bmatrix} a_{k,\lambda}, a_{k',\lambda'} \end{bmatrix} \right\}$$

$$\times e^{i\mathbf{k} \mathbf{x} - i\omega_{k}t - i\mathbf{k}' \cdot \mathbf{x}' + i\omega_{k'}t} - \begin{bmatrix} a_{k,\lambda}^{\dagger}, a_{k',\lambda'} \end{bmatrix}$$

$$\times e^{-i\mathbf{k} \cdot \mathbf{x} + i\omega_{k}t + i\mathbf{k}' \cdot \mathbf{x}' - i\omega_{k'}t} + \begin{bmatrix} a_{k,\lambda}^{\dagger}, a_{k',\lambda'}^{\dagger} \end{bmatrix}$$

$$\times e^{-i\mathbf{k} \cdot \mathbf{x} + i\omega_{k}t - i\mathbf{k}' \cdot \mathbf{x}' + i\omega_{k'}t} - \begin{bmatrix} a_{k,\lambda}^{\dagger}, a_{k',\lambda'}^{\dagger} \end{bmatrix}$$

$$\times e^{-i\mathbf{k} \cdot \mathbf{x} + i\omega_{k}t - i\mathbf{k}' \cdot \mathbf{x}' + i\omega_{k'}t} - \begin{bmatrix} a_{k,\lambda}^{\dagger}, a_{k',\lambda'}^{\dagger} \end{bmatrix}$$

$$\times e^{i\mathbf{k} \cdot \mathbf{x} - i\omega_{k}t + i\mathbf{k}' \cdot \mathbf{x}' - i\omega_{k'}t}$$
Using the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the "radiation field" and the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same set as a second of the same second of the same set as a second of the same set as a second of the same second of the

Using the commutators (65) for a_k , λ and a_k^{\dagger} we have

$$[A_{i}(\mathbf{x},t),\pi_{j}(\mathbf{x}',t)] = \frac{1}{V} \sum_{k,\lambda} \sum_{k',\lambda'} \frac{\left(\hat{\epsilon}_{k,\lambda}\right)_{i} \left(\hat{\epsilon}_{k,\lambda}\right)_{j}}{2\sqrt{(\omega_{k}\omega_{k'})}} \cdot i\omega_{k}$$

$$\times \left\{\delta_{\lambda\lambda'}\delta_{kk'}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} + \delta_{\lambda\lambda'}\delta_{kk'}e^{-i\mathbf{k}\cdot(\mathbf{x}'-\mathbf{x})}\right\}$$

$$= \frac{1}{V} \sum_{k,\lambda} \left(\hat{\epsilon}_{k,\lambda}\right)_{i} \left(\hat{\epsilon}_{k,\lambda}\right)_{j} \frac{i}{2} \left\{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} + e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\right\}$$

$$= \frac{1}{V} \sum_{k'} \left(\delta_{ij} - \frac{k_{i}k_{j}}{k^{2}}\right) \frac{i}{2} \left\{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} + e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\right\}$$

{Using eqn. (63)}

This in the limit $V \rightarrow \infty$, yields

$$[A_{i}(\mathbf{x}, t), \pi_{j}(\mathbf{x}', t)] = i \frac{1}{(2\pi)^{3}} \int \left(\delta_{jj} - \frac{k_{i}k_{j}}{k^{2}}\right) e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} d^{3}k$$

$$= i\delta_{ij}^{tr}(\mathbf{x} - \mathbf{x}')$$
Similarly we see

Similarly we can verify the other of the rules (59).

Now we find out an expression for the total hamiltonian of the field in terms of the creation and the annihilation operators. The classical expression for the total Hamiltonian is given by

$$H = \frac{1}{2} \int d^3x \ (E^2 + B^2) \qquad \dots (66)$$

We have,

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} = \frac{1}{\sqrt{(V)}} \sum_{k, \lambda} \frac{\hat{\epsilon}_{k, \lambda}}{\sqrt{(2\omega_{k})}} . i\omega_{k}$$

$$\times \left\{ a_{k, \lambda}(t) e^{i\mathbf{k} \cdot \mathbf{x}} - a_{k, \lambda}^{\dagger}(t) e^{-i\mathbf{k} \cdot \mathbf{x}} \right\}$$

and

$$B = \nabla \times A = \frac{1}{\sqrt{(V)}} \sum_{k, \lambda} \frac{i \left(\mathbf{k} + \hat{\epsilon}_{k, \lambda}\right)}{\sqrt{(2\omega_{k})}}$$

$$\times \left\{ a_{k, \lambda}(t) e^{i\mathbf{k} \cdot \mathbf{x}} - a_{k, \lambda}^{\dagger} (t) e^{-i\mathbf{k} \cdot \mathbf{x}} \right\}$$

$$\cdot \int E^{2} d^{3}x = \frac{1}{V} \sum_{k, \lambda} \sum_{k', \lambda'} \frac{\omega_{k}\omega_{k'}}{2\sqrt{(\omega_{k}\omega_{k'})}} \hat{\epsilon}_{k, \lambda} \hat{\epsilon}_{k, \lambda'}$$

$$\times \int d^{3}x \left\{ a_{k, \lambda} a_{k', \lambda'}^{\dagger} e^{i (\mathbf{k} - \mathbf{k}) \cdot \mathbf{x}} \right.$$

$$+ a_{k, \lambda}^{\dagger} a_{k', \lambda'} e^{i (\mathbf{k} - \mathbf{k}) \cdot \mathbf{x}}$$

$$- a_{k, \lambda} a_{k', \lambda'} e^{i (\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}} \right\}$$

$$= \sum_{k, \lambda} \sum_{k', \lambda'} \frac{\omega_{k}\omega_{k'}}{2\sqrt{(\omega_{k}\omega_{k'})}} \delta_{\lambda\lambda'} \left\{ a_{k, \lambda} a_{k', \lambda'}^{\dagger} e^{-i (\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}} \right\}$$

$$= \sum_{k, \lambda} \sum_{k', \lambda'} \frac{\omega_{k}\omega_{k'}}{2\sqrt{(\omega_{k}\omega_{k'})}} \delta_{\lambda\lambda'} \left\{ a_{k, \lambda} a_{k', \lambda'}^{\dagger} \delta_{k, \lambda'} + a_{k, \lambda}^{\dagger} a_{k', \lambda'}^{\dagger} \delta_{k, k'} \right.$$

$$= \sum_{k, \lambda} \frac{\omega_{k}}{2} \left(a_{k, \lambda} a_{k, \lambda}^{\dagger} + a_{k, \lambda}^{\dagger} a_{k, \lambda} - a_{k, \lambda}^{\dagger} a_{k, \lambda}^{\dagger} a_{k, \lambda}^{\dagger} a_{k, \lambda}^{\dagger} \right) \frac{1}{k'} \delta_{k, \lambda'}$$
Also, we have

Also, we have

$$i^{3}xB^{2} = \frac{1}{V} \sum_{k,\lambda} \sum_{k',\lambda'} \frac{(\mathbf{k} \times \hat{\epsilon}_{k,\lambda}) \cdot (\mathbf{k}' \times \hat{\epsilon}_{k,\lambda'})}{2\sqrt{(\omega_{k} \, \alpha_{k'})}} \int a^{3}x \left\{ a_{k,\lambda} a_{k',\lambda'}^{\dagger} e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{x}} + a_{k,\lambda}^{\dagger} a_{k,\lambda'}^{\dagger} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{x}} - a_{k,\lambda} a_{k',\lambda'}^{\dagger} e^{i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}} - a_{k,\lambda}^{\dagger} a_{k',\lambda'}^{\dagger} e^{-i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}} - a_{k,\lambda}^{\dagger} a_{k',\lambda'}^{\dagger} e^{-i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}} \right\}$$

Using the vector identity $(A \times B) \cdot (C \times D) = (A \cdot C) (B \cdot D) - (A \cdot D) (B \cdot C)$ we have,

$$(\mathbf{k} \times \hat{\epsilon}_{k}, \lambda) \cdot (\mathbf{k}' \times \hat{\epsilon}_{k}, \lambda) = (\mathbf{k} \cdot \mathbf{k}') (\hat{\epsilon}_{k}, \lambda \cdot \hat{\epsilon}_{k}, \lambda') - (\mathbf{k} \cdot \hat{\epsilon}_{k}, \lambda') (\mathbf{k}' \cdot \hat{\epsilon}_{k}, \lambda)$$

$$= (\mathbf{k} \cdot \mathbf{k}') \delta_{\lambda \lambda'}$$

{Using the orthogonality of k and $\hat{\epsilon_k}$, λ }

$$\int d^3x B^2 = \sum_{k,\lambda} \sum_{k',\lambda} \frac{(\mathbf{k} \cdot \mathbf{k'}) \, \delta_{\lambda,\lambda} \, \lambda'}{2\sqrt{(\omega_k \, \omega_{k'})}} \left(a_{k,\lambda} \, a_{k',\lambda'}^{\dagger} \, \delta_{k,k'} + a_{k,\lambda}^{\dagger} \, a_{k',\lambda'}^{\dagger} \delta_{kk}, \right.$$

$$-a_{k,\lambda}a_{k',\lambda'}\delta_{k,-k'}-a_{k,\lambda}^{\dagger}a_{k',\lambda'}\delta_{k,-k'}$$

$$=\sum_{k,\lambda}\frac{\omega_{k}}{2}\left(a_{k,\lambda}a_{k,\lambda}^{\dagger}+a_{k,\lambda}^{\dagger}a_{k,\lambda}^{\dagger}+a_{k,\lambda}^{\dagger}a_{-k,\lambda}^{\dagger}+a_{k,\lambda}^{\dagger}a_{-k,\lambda}^{\dagger}\right)$$
...(68)

Using (67) and (68) in (66) we get:

$$\begin{split} H &= \frac{1}{2} \sum_{k, \lambda} \frac{\omega_{k}}{2} \left(2a_{k, \lambda} a_{k, \lambda}^{\dagger} + 2a_{k, \lambda}^{\dagger} a_{k, \lambda} \right) \\ &= \sum_{k, \lambda} \omega_{k} \left(a_{k, \lambda}^{\dagger} a_{k, \lambda} + \frac{1}{2} \right) \left\{ \vdots \quad a_{k, \lambda} a_{k, \lambda}^{\dagger} - a_{k, \lambda}^{\dagger} a_{k, \lambda} = 1 \right\} \end{split}$$

Defining the particle number operator N_k , $\lambda = a_k^{\dagger}$, $\lambda^a k$, λ^a for the photons, we have

$$H = \sum_{k, \lambda} \omega_k (N_k, \lambda + \frac{1}{2}) \qquad \dots (69)$$

The number operator N_k , λ has the eigenvalues 0, 1, 2, 3,..... The creation and the annihilation operators can be interpreted in the same manner as that for the scalar field,

$$a_{k,\lambda} \mid n_{k,\lambda} \rangle = \sqrt{(n_{k,\lambda}) \mid n_{k,\lambda} - 1 \rangle}$$

$$a_{k,\lambda}^{\dagger} \mid n_{k,\lambda} \rangle = \sqrt{(n_{k,\lambda} + 1) \mid n_{k,\lambda} + 1 \rangle}$$

$$\dots (70)$$

1.1.6. QUANTIZATION OF PROCA'S FIELD:

As we remarked in the classical theory of fields, the Quantized Proca's Field describes some sort of mesons of spin one and non-

vanishing rest mass. However, there is no evidence for the existence of such particles and hence the quantization of Proca's field is of theoretical importance only. Proca's Field can very easily be quantized by the usual method of canonical quantization. In PROBLEM-7 of the last chapter we have seen that the component π_4 of the momentum vanishes identically, therefore, V_4 will commute with all the other components of the field operators and hence it is just a classical number and not an operator and therefore, it is of no physical significance in the quantization of the field. V_4 is the redundant component and it may be eliminated from V_{μ} . The equal time commutators for π_i and V_i can be written by the canonical procedure as:

$$[V_i(\mathbf{x},t),V_j(\mathbf{x}',t)] = [\pi_i(\mathbf{x},t),\tau_j(\mathbf{x}',t)] = 0 \qquad ...(71a)$$

$$[V_i(\mathbf{x}, t), \pi_j(\mathbf{x}', t)] = i\delta_{ij} \,\delta^3(\mathbf{x} - \mathbf{x}') \qquad ...(71b)$$

We can proceed without ever bringing in the components V_4 and π_4 , because they play no role in the field dynamics. The quantized field V can be expanded in terms of creation and annihilation operators as:

$$V(\mathbf{x}, t) = \frac{1}{\sqrt{(V)}} \sum_{k}^{1} \frac{1}{\sqrt{(2\alpha_{k})}} \sum_{\lambda=1}^{\hat{e}_{k,\lambda}} \left[a_{k,\lambda}(t) \exp(i\mathbf{k} \cdot \mathbf{x}) + a_{k,\lambda}^{\dagger}(t)(\exp(-i\mathbf{k} \cdot \mathbf{x})) \right] \dots (72)$$

where the creation and the annihilation operators $a_{k,\lambda}^{\dagger}(t)$ and $a_{k,\lambda}(t)$ satisfy the following commutation rules

$$\left[a_{k,\lambda}(t), a_{k',\lambda'}^{\dagger}(t)\right] = \delta_{kk'} \delta_{\lambda\lambda'} \qquad \dots (73)$$

with all other commutators between a_k , and a_k^{\dagger} , as vanishing.

The polarization vectors e are normalized such that

$$\sum_{\lambda=1}^{3} (\hat{e}_{k,\lambda})_{i} (\hat{e}_{k,\lambda})_{j} = \left(\delta_{ij} + \frac{k_{i} k_{i}}{m^{2}} \right)$$

$$\sum_{\lambda=1}^{3} (\hat{e}_{k,\lambda})_{i} (\hat{a}_{k,\lambda}')_{i} = \delta_{\lambda\lambda}'$$

$$\vdots = 1 \qquad (74)$$

or

A solution may be written in the sorm

$$(e_{k,\lambda})_{i} = \delta_{i\lambda} + \alpha k_{i}k_{\lambda} \qquad ...(75)$$

$$(\delta_{i\lambda} + \alpha k_{i}k_{\lambda}) (\delta_{j\lambda} + \alpha k_{j}k_{\lambda}) = \delta_{ij} + \frac{k_{i} k_{j}}{m^{2}} \Rightarrow$$

$$2\alpha k_{i} k_{j} + \alpha^{2}k_{i} k_{j}k^{2} = \frac{k_{i}k_{j}}{m^{2}}$$

$$2\alpha + \alpha^{2}k^{2} = \frac{1}{m^{2}}$$

 $\alpha = \frac{1}{m(\omega_k + m)} \quad \text{or} \quad \frac{1}{m(\omega_k - m)} \quad \{: \omega_k^2 = k^2 + m^2\}$

Taking the positive sign,

$$(\hat{e}_{k},_{\lambda})_{i} = \delta_{i\lambda} + \frac{k_{i}k_{\lambda}}{m(\omega_{k} + m)} \qquad ...(76)$$
we have all integrals

Though we have eliminated the component V_4 in the quantized Proca's field, yet the sake of Lorentz covariance, it is better to write

$$V_{\mu} = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \sum_{\lambda=1}^{3} (e_{k,\lambda})_{\mu} \left[a_{k,\lambda}(0) \exp. (ik.x) + a_{k,\lambda}^{\dagger}(0) \exp. (-ik.x) \right]$$
and the polarization sum

$$\sum_{\lambda=1}^{3} (e_{k,\lambda})_{\mu} \cdot (e_{k,\lambda})_{\nu} = \left(\delta_{\mu\nu} + \frac{k_{\mu}k_{\nu}}{m^2}\right) \dots (78)$$

The construction of the Fock-space for Proca's field proceeds completely analogous to those for the Maxwell's field.

13.7. INTERACTION BETWEEN FIELDS:

In the preceding sections we have quantized the various fields in the free state *i.e.* without any interaction with other fields. A theory of free fields alone has no physical content. The importance of the quantized fields is revealed to us through the interactions between the free fields. We have seen that a quantized free field represents a system of particles; e.g. quantized Dirac field represents the electrons and the Maxwell's field when quantized represents photons. The interaction between two fields is actually the interaction between the two system of particles represented by those fields. The Lagrangian for mutually interacting fields must contain terms constructed from field functions

of both the fields. Thus the Lagrangian density for a system of two interacting fields can be written as:

 $L = L_1 + L_2 + L_{Ini}. \qquad ...(79)$

where L₁ and L₂ are free field Lagrangians and L_{Int}, is the interaction term which depends on both the fields. The explicit form of the L_{Int}, depends on the type of the fields and the nature of the interaction, however the general conditions to be satisfied by it are:

- (i) L_{Int}. should be Hermitian. Since all physical variables like energy, momentum, etc. are derivable from the Lagrangian, and since a physical observable must be real, this necessitates the Hermiticity of L and therefore of L_{Int}.
- (ii) L_{Int} should be invariant. This guarentees the Lorentz-covariance of coupled field equations.
- (iii) L_{Int} should be local, i e., it must be determined by both the field variables taken at the same point x. A non-local interaction can be written as

 $L_{Int.} = \int F(x, x') f(\psi(x), \varphi(x')) dx'$...(80)

where F(x, x') is a form factor characterizing the spread out of the interaction zone. For a local theory there is no action at a distance so that $F(x, x') = \delta(x - x')$. When L_{Int} is local it satisfies the condition of causality. The instantaneous interaction at a distance being absent, there is no violation of the principle that a signal cannot propagate with a velocity greater than that of light.

The general form of the interaction between two fields is written as f(x) g(x), where f(x) stands for the contribution due to the first field and g(x) for the contribution due to the second field. If none of f(x) and g(x) involves the derivative of the field functions we, call the interaction as 'Direct one' and if derivatives are involved, the coupling is known as 'Derivative one'.

Our field functions are normalized by virtue of the expression for the lagrangian of the free fields. The strength of the interaction term in the lagrangian is measured by the magnitude of a real multiplicative factor, called the *Coupling Constant*.

Using the above guidelines, now write the interaction term for the interaction of the Dirac field with other fields. For the interaction with the scalar field $\varphi(x)$, in the direct type of coupling, we set $f(x) = \varphi(x)$ and form a scalar covariant $g(x) = \psi(x) \psi(x)$ so that the covariant interaction term becomes:

$$G\psi(x) \psi(x) \varphi(x)$$

For the derivative type of coupling, we set $f(x) = \partial_{\mu} \varphi(x)$ and for g(x) we take the vector covariant ' $\psi(x) \gamma_{\mu} \psi(x)$ ' formed from $\psi(x)$. We use F/m for the coupling canstant, with m as the mass of the particle of the field $\varphi(x)$, and F is then dimensionless. Hence the invariant interaction term becomes:

$$\frac{F}{m} \overline{\psi}(x) \gamma_{\mu} \psi(x) \partial_{\mu} \varphi(x) \qquad ...(81)$$

Now we write the interaction with a vector field $A_{\mu}(x)$. In the direct coupling we combine the vector $A_{\mu}(x)$ with the vector covariant $\psi(x) \gamma_{\mu} \psi(x)$ and obtain the interaction term

$$G\psi(x) \gamma_{\mu} \psi(x) A_{\mu}(x)$$
 ...(82)

The usual relativistic convention of summation over μ is implied in (81) and (82). In the derivative coupling, the interaction term involves the derivative $\frac{\partial A_{\mu}}{\partial x_{\nu}}$. We assume that the vector field A_{μ} is of the type of the Maxwell's field and the field equations involve only the antisymmetric tensor $F_{\mu\nu}$, Hence it is useful to introduce $F_{\mu\nu}$ in the derivative coupling with Dirac field. For this purpose we combine $F_{\mu\nu}$ with the antisymmetric tensor covariant $\psi \sigma_{\mu\nu} \psi$ and obtain

$$\frac{F}{m} \overline{\psi} \sigma_{\mu\nu} \psi F_{\mu\nu} = \frac{F}{2im} \overline{\psi} \left(\gamma_{\mu} \gamma_{\nu} - \gamma_{\nu} \gamma_{\mu} \right) \psi F_{\mu\nu}.$$

$$11NEOUAL TIME. (83)$$

13.8. UNEQUAL TIME COMMUTATORS:

We have quantized the free fields by defining equal time commutators for the field parameters. The quantization by equal time commutators does not loose any information as far as the free fields are concerned. But for the interacting fields, these commutation relations are not adequate. In order to exhibit the relativistic invariance of the theory for the interacting fields, we have to consider the unequal time commutators. This is possible in brief.

REAL SCALAR FIELD:

First we consider the case of the real scalar (Boson) field. In the Schroedinger representation, the time-independent field operator $\phi(x)$ has the following expansion in terms of the creation and annihilation operators $a_{\uparrow k}^{-}(t)$ and $a_k^{-}(t)$:

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2w_k)}} \left[a_k(t) \exp_{-ik}(i\mathbf{k}.\mathbf{x}) + a\dagger k(t) \exp_{-ik}(-i\mathbf{k}.\mathbf{x}) \right] \dots (84)$$

where $[a_k(t), a_{k'}^{\dagger}(t)] = \delta_{kk''}$...(85a)

$$[a_k(t), a_{k'}(t)] = \left[a_k^{\dagger}(t), a_{k'}^{\dagger}(t) \right] = 0 \qquad ...(85b)$$

In order to find the field operator ϕ (x, t) of the interaction picture, we need to find the explicit time dependence of the operators a_k (t) and a_k [†](t). For it we have, from eqn. (83) of chapter (3), as

 $a_k(t) = \exp(iH_0t) a_k(0) \exp(-iH_0t)$...(86)

(In what follows we shall be writing a_k for a_k (0).)

with
$$H_0 = \sum_k N_k \ \omega_k = \sum_k a_k^{\dagger} a_k \ \omega_k$$
 ...(87)

Since a_k commutes with a_k^{\dagger} , $a_{k'}$ for $k \neq k'$, therefore, it is sufficient to consider

$$a_k(t) = \exp\left(ia_k^{\dagger} a_k \omega_k t\right) a_k \exp\left(-ia_k^{\dagger} a_k \omega_k t\right)$$

To simplify this expression we write

$$a_k(\lambda) = \exp\left(ia_k^{\dagger} a_k a_k t\lambda\right) a_k \exp\left(-ia_k^{\dagger} a_k \omega_k t\lambda\right) \dots (88)$$

so that

or

$$a_k(1) = a_k(t) \text{ and } a_k(0) = a_k.$$

Differentiating (88) w.r.t. \(\lambda\), we obtain

$$\frac{da_k}{d\lambda} = \exp. (iN_k \omega_k t \lambda) i\omega_k t [N_k, a_k] \exp. (-iN_k \omega_k t \lambda)$$

$$= -i\omega_k t a_k (\lambda) \qquad ...(89)$$

[It is left as an exercise for the readers to verify this relation] Integrating (89) with the initial condition $a_k(\lambda) = a_k(0)$ for $\lambda = 0$, we get, $a_k(\lambda) = a_k(0)$ exp. $(-i\omega_k + \lambda)$

$$a_{k}(1) = a_{k}(0) \exp(-i\omega_{k}t)$$

$$a_{k}(t) = a_{k} \exp(-i\omega_{k}t)$$

$$\{ :: a_{k}(1) = a_{k}(+) \}$$

A similar computation for the creation operator yields

$$a_{li}^{\dagger}(t) = a_{li}^{\dagger} \exp. (i\omega_{li}t)$$
 ...(89b)

Using (89a and b) we can write (84) as:

$$\phi(\mathbf{x},t) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left[a_{k} \exp_{\cdot} (i\mathbf{k} \cdot \mathbf{x} - i\omega_{k}t) + a_{k}^{\dagger} \exp_{\cdot} (-i\mathbf{k} \cdot \mathbf{x} + i\omega_{k}t) \right]$$

$$= \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_{k})}} \left(a_{k} e^{ik\cdot x} + a_{k}^{\dagger} e^{-ik\cdot x} \right) ...(90)$$

From the equal time commutation rules (85) we can easily derive the unequal time commutators, using the interaction representation (90). We have

$$[\phi(\mathbf{x},t), \phi(\mathbf{x}',t')] = \frac{1}{V} \sum_{k,k'} \frac{1}{2\sqrt{(\omega_k \omega_{k'})}} \left\{ [a_k, a_{k'}] \exp_{\cdot} [i(k.x+k'.x')] + \left[a_k, a_{k'}^{\dagger} \right] \exp_{\cdot} [i(k.x+k'.x')] + \left[a_k^{\dagger}, a_{k'}^{\dagger} \right] \exp_{\cdot} [-i(k.x-k'.x')] + \left[a_k^{\dagger}, a_{k'}^{\dagger} \right] \exp_{\cdot} [-i(k.x+k'.x')] + \left[a_k^{\dagger}, a_{k'}^{\dagger} \right] \exp_{\cdot} [-i(k.x+k'.x')] + \left[a_k^{\dagger}, a_{k'}^{\dagger} \right] \exp_{\cdot} [-i(k.x+k'.x')]$$

{Using commutators (85)}

Putting (x-x')=y, we can write.

$$[\phi(\mathbf{x},t),\phi(\mathbf{x}',t')] = \frac{1}{V} \sum_{k} \frac{1}{2\omega_{k}} [e^{ik\cdot y} - e^{-ik\cdot y}] \qquad ...(91)$$

We can change the summation on the right hand side of eqn. (91) into an integration by the standard prescription

$$\frac{1}{V} \sum_{k} f(\mathbf{k}) \longleftrightarrow \frac{1}{(2\pi)^3} \int d^3k \, f(\mathbf{k}) \qquad \dots (92)$$

If we define the quantity $\triangle(y)$ by

$$\Delta(y) = -\frac{i}{(2\pi)^8} \int \frac{d^3k}{2\omega_k} \left(e^{iky} - e^{-iky}\right)$$

$$= -\frac{1}{(2\pi)^3} \int \frac{d^3k}{\omega_k} \exp. (i\mathbf{k} \cdot \mathbf{y}) \sin k_0 y_0, \qquad ...(93)$$

then the commutation rule (91) can be written as

$$[\phi(\mathbf{x},t),\phi(\mathbf{x}',t')]=i\Delta(y)=i\Delta(x-x') \qquad ...(94)$$

The function $\triangle(y)$, called the Pauli-Jordan \triangle -function has the following important properties:

- 1. It is Lorentz invariant under all ordinary Lorentz transformations (without time reflection).
- 2. $\triangle(x-x')$ vanishes for $x_0=x'_0$ i.e. for equal times. Thus we see from (94) that the equal time commutators of two field amplitudes vanishes, as required. This property of \triangle -function easily follows from its definition (93).
- 3. $\triangle(y)=0$ for $y^2>0$ (space like distances). This follows from relativistic invariance; since by a suitable Lorentz transformation we can always transform to a new frame in which $y_0=0$; i.e. $x_0-x'_0=0$ or $x_0=x'_0$. It then follows from property 2.
- 4. $\triangle(y)$ is an odd function, i.e. $\triangle(-y) = -\triangle(y)$. This property follows readily from the definition of $\triangle(y)$.

5.
$$\frac{\partial \Delta(y)}{\partial y_0}\Big|_{y_0=0} = -\delta^3(y) \text{ or } \frac{\partial \Delta(x-x')}{\partial x_0}\Big|_{x=x'_0} = -\delta^3(x-x')$$

To show this, from the definition eqn. (93) of $\Delta(y)$ we have

$$\frac{\partial \triangle(y)}{\partial y_0} = -\frac{1}{(2\pi)^3} \int d^3k \exp. (i\mathbf{k} \cdot \mathbf{y}) \cos k_0 y_0$$

$$\{ :: k_0 = \omega_k \}$$

$$\frac{\partial \triangle(y)}{\partial y_0} \Big|_{y_0 = 0} = -\frac{1}{(2\pi)^3} \int d^3k \exp. (i\mathbf{k} \cdot \mathbf{y}) = -\delta^3 (\mathbf{y})$$

Since y=x-x', we can also write it as

$$\frac{\partial \Delta(x-x')}{\partial x_0}\Big|_{x_0 = x_0'} = -\delta^3 (x-x')$$

It should be noted that our equal time commutation rule for $\pi(x)$ and $\phi(x)$ (see eqn. 7) follows from equation (94) using this property of $\Delta(y)$. We have

$$\pi(\mathbf{x}, t) = \frac{\partial \varphi(\mathbf{x}, t)}{\partial x_0} \quad \{ : x_0 = t \text{ in natural units} \}$$

Hence we can write,

$$[\phi(\mathbf{x}), \pi(\mathbf{x}')] = [\phi(\mathbf{x}, t), \pi(\mathbf{x}', t')]_{t=t'}$$

$$= [\phi(\mathbf{x}, t), \pi(\mathbf{x}', t')]_{x0=x0'}$$

$$= -\left\{ \frac{\partial}{x_0} \left[\phi(\mathbf{x}, t), \phi(\mathbf{x}', t') \right] \right\}_{x_0 = x_0'}$$

$$= -i \frac{\partial \Delta(\mathbf{x} - \mathbf{x}')}{x_0} \Big|_{x_0 = x_0'}$$

$$= i \delta^3(\mathbf{x} - \mathbf{x}')$$

6. $\triangle(y)$ satisfies the Klein-Gordon equation, $(\square_x - m^2) \triangle(y) = 0$

This can very easily be proved from the fact that the field variable $\phi(x)$ satisfies the Klein-Gordon equation,

$$(\square_x - m^2) \triangle (x - x');$$

as follows:

$$(\Box_{x}-m^{2}) \triangle(y) = (\Box_{x}-m^{2}) \triangle(x-x')$$

$$= (\Box_{x}-m^{2}) [\phi(x), \phi(x')]$$

$$= [(\Box_{x}-m^{2}) \phi(x), \phi(x')]$$

$$= [0, \phi(x')] = 0$$

Since $\triangle(y)$ satisfies a secand order differential equation, it can be uniquely determined from the two initial conditions at $y_0=0$,

 $\Delta(y)\Big|_{y_0=0}=0 \text{ and } \frac{\partial \Delta(y)}{\partial y_0}\Big|_{y_0=0}=-\delta(y).$

From eqn. (90) it is clear that the frequency dependences of the creation and the destruction parts of $\phi(x, t)$ are different, because $\omega_k = \sqrt{(k^2 + m^2)}$ is positive. Thus we can decompose $\phi(x)$ into a positive and a negative frequency part as

$$\phi(x) = \phi^{(+)}(x) + \phi^{(-)}(x) \qquad ...(95)$$

X

where

$$\phi^{(+)} = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_k)}} a_k e^{ik \cdot \pi} \qquad \dots (96a)$$

and

$$\phi^{(-)}(x) = \frac{1}{\sqrt{(V)}} \sum_{k} \frac{1}{\sqrt{(2\omega_k)}} a_{s}^{\dagger} e^{-ik \cdot x} \qquad ...(96b)$$

From these eqns. we find that

$$[\phi^{(-)}(x)]\dagger = \phi^{(+)}(x) \qquad ...(97)$$

The operator $\phi^{(+)}(x)$ is a destruction operator and $\phi^{(-)}(x)$ is a creation operator.

The vacuum state which was previously characterized by $a_k \mid 0 > = 0$, for all k, can be defined, now, as

$$\phi^{(+)}(x) \mid 0 \rangle = 0 \qquad ...(98)$$

In our later work we shall have situations to use the commutation rules between $\phi^{(+)}(x)$ and $\phi^{(-)}(x)$. These, by virtue of (85) and (96), are

...(99a) $[\phi^{(\pm)}(x), \phi^{(\pm)}(x')] = 0$

and

$$[\phi^{(\pm)}(x), \phi^{(\mp)}(x')] = \frac{\pm 1}{(2\tau)^3} \int \frac{d^3k}{2\omega_k} e^{\pm ik \cdot y}$$

$$= i\triangle^{(\pm)}(y) \qquad ...(99b)$$

In the above, either we take the the upper or the lower sign throughout.

It is clear from the above definitions of $\triangle^{(+)}$ and $\triangle^{(-)}$ that

$$\Delta(y) = \Delta^{(+)}(y) + \Delta^{(-)}(y) \qquad ...(100)$$

We also define another invariant function, (1) satisfies the Klein-Gordon equation but which is an even function.

$$\triangle^{(1)}(y) = \triangle^{(+)}(y) - \triangle^{(-)}(y)$$

$$= -\frac{i}{(2\pi)^3} \int \frac{d^3k}{\omega_k} \exp.(i\mathbf{k} \cdot \mathbf{y}) \cos k_0 y_0...(101)$$

The function $\Delta^{(1)}$ occcurs when we take the vacuum expectation value of the anticommutator $[\phi(x), \phi(x')]_{+}$. Thus using the definition of the vacuum, Eqn. (98), and the adjoint property (97), we find that

we find that
$$\langle 0 \mid [\phi(x), \phi(x')]_{+} \mid 0 \rangle = \langle 0 \mid \langle \phi(x) \phi(x') + \phi(x') \phi(x) \rangle \mid 0 \rangle$$

$$= \langle 0 \mid \phi^{(+)}(x) \phi^{(-)}(x') + \phi^{(+)}(x') \phi^{(-)}(x) \mid 0 \rangle$$

$$= \langle 0 \mid \{ [\phi^{(+)}(x), \phi^{(-)}(x')] + [\phi^{(+)}(x'), \phi^{(-)}(x)] \} \mid 0 \rangle$$

$$= \langle 0 \mid \{ i\Delta^{(+)}(x - x') + i\Delta^{(+)}(x' - x) \} \mid 0 \rangle$$

$$= \langle 0 \mid \{ i\Delta^{(+)}(x - x') - i\Delta^{(-)}(x - x') \} \mid 0 \rangle$$

$$= \langle 0 \mid \{ i\Delta^{(+)}(x - x') - i\Delta^{(-)}(x - x') \} \mid 0 \rangle$$

$$= \langle 0 \mid \{ i\Delta^{(+)}(y) - \Delta^{(-)}(y) \}$$

$$= i \{ \Delta^{(+)}(y) - \Delta^{(-)}(y) \}$$

$$= i \{ \Delta^{(1)}(y) \qquad \dots (102) \}$$

DIRAC'S FIELD:

Now we find out the unequal time commutators for the Dirac The field functions are expanded in terms of the creation and annihilation operators as

$$\psi(\mathbf{x}) = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} \left[b_{rp}(t) u^r(\mathbf{p}) \exp. (i\mathbf{p} \cdot \mathbf{x}) + d_{rp} \dagger(t) v^r(\mathbf{p}) \exp. (-i \cdot \mathbf{x})\right]$$

As in the case of the Boson field, the explicit time dependence of the operators $b_{rp}(t)$ and $d_{rp}(t)$ is given by:

 $b_{rp}(t) = b_{rp}(0) \exp \{-E_p t\}, \text{ and } d_{rp}(t) = d_{rp}(0) \exp \{-E_p t\} \dots (103)$

Hence we can write,

$$\psi(x) = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} \left[b_{rp} u^r (p) \exp. \{ip.x\} + d_{rp}^{\dagger} v^r (p) \exp. \{-ip.x\} \dots (104) \right]$$

Here we denote $b_{rp}(0)$ and $d_{rp}(0)$ by b_{rp} and $d_{rp}.p$ is the energy-momentum four-vector the components (p, iE_p) and $E_p = \sqrt{(p^2 + m^2)}$.

Equation (104) can be splitted into the positive and negative energy parts as:

$$\psi(x) = \psi^{(+)} + \psi^{(-)} \qquad ...(105)$$

where

$$\psi^{(+)} = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} b_{rp} u^r (p) \exp. \{ip \cdot x\} \dots (106a)$$

is the destruction operator for a fermion, and

$$\psi^{(-)} = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} d_{r_p}^{\dagger} v^r (\mathbf{p}) \exp. \{-ip.x\} \dots (106b)$$

is the creation operator for an antifermion

From (104) we have,

$$\overline{\psi}(x) = \frac{1}{\sqrt{(V)}} \sum_{r,p} \left[\sqrt{\left(\frac{m}{E_p}\right)} \left[b_{rp}^{\dagger} \overline{u}^r (p) \exp. \{-ip.x\} \right] \right]$$

$$+d_{rp}\bar{v}^{r}$$
 (p) exp. $\{ip \cdot x\}$ $= \bar{\psi}^{(-)} + \bar{\psi}^{(+)}$...(107)

where

$$\overline{\psi}^{(-)} = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} b_{rp}^{\dagger} \overline{u}^r \text{ (p) exp. } \{-ip.x\} \qquad \dots (108a)$$

is the creation operator for a fermion, and

$$\bar{\psi}^{(+)} = \frac{1}{\sqrt{(V)}} \sum_{r, p} \sqrt{\left(\frac{m}{E_p}\right)} d_{rp} \bar{v}^r \text{ (p) exp. } \{ip.x\} \qquad ...(108b)$$

is the destruction operator for an antifermion.

From eq. (106) and (108) it follows that

$$\overline{\psi_{\alpha}^{(-)}} = \overline{\psi_{\alpha}^{(+)}}$$
 and $\overline{\psi_{\alpha}^{(+)}} = \overline{\psi_{\alpha}^{(-)}}$

The operators b_{rp} and d_{rp} satisfy the following commutation rules,

$$\left[\begin{array}{c} b_{rp}, b_{r'p'}^{\dagger} \end{array}\right]_{+} = \left[\begin{array}{c} d_{rp}, d_{r'p'}^{\dagger} \end{array}\right]_{+} = \delta_{rr'} \delta_{p,r'} \qquad ...(i09)$$

with all the other anticommutators between these operators as vanishing. Using these anti-commutators we find that:

$$[\psi^{(+)}x_{,},\psi^{(-)}(x')]_{+} = [\psi^{(-)}(x),\psi^{(+)}(x')]_{+} = 0$$
 ...(110)
$$[\psi^{(+)}(x),\psi^{(+)}(x')]_{+} = [\psi^{(-)}(x),\psi^{(-)}(x')]_{+} = 0$$

whereas,

$$\psi_{\alpha}^{(+)}x, \bar{\psi}_{\beta}^{(-)}(x')]_{+} = \frac{1}{V} \sum_{r, p} \frac{m}{E_{p}} \exp. \{ip.(x-x')\}$$

$$\times \left[b_{r\,p}, b_{r\,p}^{\dagger} \right]_{+} u^{r}_{\alpha}(\mathbf{p}) \bar{u}^{r}_{\beta} (\mathbf{p})$$

$$= \frac{1}{V} \sum_{p} \frac{m}{E_{p}} \exp. \{ip. (x-x') \sum_{r} u_{\alpha}^{r} (\mathbf{p}) \bar{u}_{\beta}^{r} (\mathbf{p})$$

$$= \frac{1}{V} \sum_{p} \frac{m}{E_{p}} \exp. \{ip. (x-x') \Lambda^{(+)}_{\alpha\beta} (p)$$

where $\Lambda^{(+)}(p) = \frac{m-ip}{2m}$ is the positive energy projection operator.

Changing the summation into the integration we can write the above eq. as:

$$[\psi_{\alpha}^{(+)}(x), \psi_{\beta}^{(-)}(x')]_{+} = \frac{1}{(2\pi)^{3}} \int_{2E_{p}}^{d^{3}p} \exp. \{ip.y\} (m-i\gamma.p)_{\alpha\beta}$$

where we have put $(x-x')=y$.

or we have,

$$[\psi_{\alpha}^{(+)}(x), \bar{\psi}_{,i}^{(-)}(x')]_{+} = \frac{1}{(2\pi)^{3}} (m - \gamma \partial_{y})_{\alpha\beta} \int_{2E_{p}}^{d^{3}p} \exp \{ip.y\}$$

$$= i(m - \gamma \partial_{y})_{\alpha\beta} \triangle^{(+)}(y)$$

$$= iS^{+}_{\alpha\beta}(y) \qquad ...(111)$$

where we define,

$$S_{\alpha\beta}^{(+)}(y) = (m - \gamma \partial_y)_{\alpha\beta} \triangle^{(+)}(y) \qquad \dots (112)$$

A similar procedure for the antiparticle operators yields

$$[\psi_{\alpha}^{(-)}(x), \psi_{\beta}^{(+)}(x')]_{+} = iS_{\alpha\beta}^{(-)}(y) \qquad ...(113)$$

where

$$S_{\alpha\beta}^{(-)}(y) = (m - \gamma \partial_y)_{\alpha\beta} \triangle^{(-)}(y) \qquad \dots (114)$$

Using eqn. (105) and (107) and the anticommutators (110), (111) and (113) we can derive the anticommutator:

$$[\psi_{\alpha}(x), \psi_{\beta}(x')]_{+} = iS_{\alpha\beta}(x - x') \qquad ...(115)$$

where

$$S_{\alpha\beta} = S_{\alpha\beta}^{(+)} + S_{\alpha\beta}^{(-)}$$

$$= (m - \gamma \partial)_{\alpha\beta} \triangle \qquad ...(116)$$

As in the case of the Boson field, here also, the equal time anticommutators can be derived from the equation (115). We have:

$$\begin{bmatrix} \psi_{\alpha}(x), \bar{\psi}_{\beta}(x') \end{bmatrix}_{+} |_{x_{0} = x_{0}'} = -(\gamma_{4})_{x\beta} \partial_{0} \triangle(x - x') |_{x_{0} = x_{0}'} \\
= (\gamma_{4})_{x\beta} \delta^{3}(x - x') \qquad \dots (117)$$

(Using property 5 of △ function)
Multiplying (117) throughout by γ_4 we get:

$$\left[\begin{array}{ccc} \psi_{\alpha}(x), \psi_{\beta}^{\dagger}(x') \end{array}\right]_{+} \Big|_{x_{0}=x_{0}'} = \delta_{\alpha\beta} \delta^{3}(x-x')$$

which is the required equal time anticommutator for the Dirac field.

Analogous to the scalar-function \triangle (y) of the Boson-field, the scalar-function S (y) of the Dirac field satisfies the Dirac equation as shown below:

$$(m+\gamma\partial_y) S(y) = (m+\gamma\partial_y)(m-\gamma\partial_y) \triangle(y)$$

$$= (m^2 - \partial_y^2) \triangle(y)$$

$$= -(\Box_y - m^2) \triangle(y) = 0$$

Thus we see that the discussion of the Dirac sield is exactly parallel to the Boson field. Therefore here also we find the vacuum expectation value of the commutators.

The vacuum state which was previously defined as $d \mid 0 \rangle = 0$,

$$b\mid 0\rangle = 0$$
 and $\langle 0\mid d^{\dagger}=0$, $\langle 0\mid b^{\dagger}=0$, can now be defined by:

$$\psi^{(+)}(x) \mid 0 \rangle = 0, \ \bar{\psi}^{(+)}(x) \mid 0 \rangle = 0, \ \langle 0 \mid \psi^{(-)}(x) = 0 \text{ and } \\ \langle 0 \mid \bar{\psi}^{(-)}(0) = 0. \\ \vdots \quad \langle 0 \mid [\psi_{\alpha}(x), \bar{\psi}_{\beta}(x')] \mid 0 \rangle = \langle 0 \mid [\{\psi_{\alpha}^{(+)}(x) + \psi_{\alpha}^{(-)}(x)\}, \\ \{\bar{\psi}_{\beta}^{(+)}(x') + \bar{\psi}_{\beta}^{(-)}(x')\}] \mid 0 \rangle \\ = \langle 0 \mid \{\{\psi_{\alpha}^{(+)}(x)\bar{\psi}_{\beta}^{(-)}(x') - \bar{\psi}_{\beta}^{(+)}(x')\psi_{\alpha}^{(-)}(x) \mid 0 \rangle \\ = \langle 0 \mid \{[\psi_{\alpha}^{(+)}(x), \bar{\psi}_{\beta}^{(-)}(x')]_{+} - [\bar{\psi}_{\beta}^{(+)}(x'), \bar{\psi}_{\alpha}^{(-)}(x)]_{+}\} \mid 0 \rangle \\ = \langle 0 \mid iS_{\alpha\beta}^{(+)}(x - x') - iS_{\alpha\beta}^{(-)}(x - x') \mid 0 \rangle \\ = iS_{\alpha\beta}^{(1)}(x - x') \qquad ...(118)$$
The $S_{\alpha\beta}^{(1)}(x - x') = S_{\alpha\beta}^{(+)}(x - x') - S_{\alpha\beta}^{(-)}(x - x') \qquad ...(119)$

Hence it is clear that all the equations of the Boson field and that of the Dirac field are analogous. The only difference in the discussion is that the role the commutator and that of the anti-commutator is interchanged.

MAXWELL'S FIELD:

To close this section, we now discuss the unequal time commutators for the Maxwell's E. M. Field. For it we note that the e.m. field is a Boson field with rest mass m=0. An argument, similar to that leading to equ. (94) for the Boson field, now indicates that the covariant unequal time commutators for the e.m. field are given by:

 $[A_{\mu}(x), A_{\nu}(x')] = i\delta_{\mu\nu} D(x-x') \qquad \dots (120)$ where D(x-x') is equal to $\Delta(x-x')$ with m=0.

$$D(y) = \frac{-i}{(2\pi)^3} \int \frac{d^3k}{2 |\mathbf{k}|} [\exp \{ik.y\} - \exp \{i(k.y)\}]$$

$$= \frac{1}{2} \cdot \frac{-i}{(2\pi)^3} \int |\mathbf{k}| d| \mathbf{k} |d\Omega [\exp \{(i\mathbf{k}.\mathbf{y} - k_0 y_0)\}]$$

$$- \exp \{i(-\mathbf{k}.\mathbf{y} - k_0 y_0)\}]$$

Carrying out the angular integration we get:

$$D(y) = \frac{1}{2} \cdot \frac{-i}{(2\pi)^3} \int_0^{\infty} |\mathbf{k}| d| \mathbf{k} |$$

$$\times \left[\frac{2\pi (\exp. \{i \mid \mathbf{k} \parallel \mathbf{y} \mid -\exp. \{-i \mid \mathbf{k} \parallel \mathbf{y} \mid \cdot \exp. \{ik_0 y_0\}\} - \frac{2\pi (\exp. \{i \mid \mathbf{k} \parallel \mathbf{y} \mid \} - \exp. \{i \mid \mathbf{k} \parallel \mathbf{y} \mid \})}{i \mid \mathbf{k} \parallel \mathbf{y} \mid} \exp. \{ik_0 y_0\} \right]$$

$$= \frac{-1}{|\mathbf{y}| 8\pi^2} \int_0^{\infty} d| \mathbf{k} | [\exp. \{(i \mid \mathbf{y} \mid -iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid \mathbf{k} \mid \} - \exp. \{(-i \mid \mathbf{y} \mid +iy_0) \mid +iy_0) \mid \}$$

Here we have replaced k_0 by $|\mathbf{k}|$ because m=0.

In order to evaluate this integral we use an arbitrary damping factor exp. $\{-k \mid \epsilon\}$ which vanishes in the large momentum limit. Hence,

$$D(y) = \frac{-1}{|\mathbf{y}|} \frac{1}{8\pi^2} \int_0^{\infty} d |\mathbf{k}| \exp \{-|\mathbf{k}| \epsilon\} [\exp \{(i |\mathbf{y}| iy_0) |\mathbf{k}| - \exp \{(-i |\mathbf{y}| - iy_0) |\mathbf{k}|\} - \exp \{(i |\mathbf{y}| + iy_0) |\mathbf{k}| + \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp \{(-i |\mathbf{y}| + iy_0) |\mathbf{k}|\} - \exp$$

Now using the relation $\frac{1}{a \pm i\epsilon} = P \frac{1}{a} \mp i\pi \delta(a)$,

where P stands for the principal value, we have:

$$D(y) = \frac{i}{4\pi^2} (-2i\pi \delta (|\mathbf{y}|^2)) = \frac{\delta (|\mathbf{y}|^2)}{2\pi} \qquad \dots (121)$$

Thus we see that D(y) has a δ -function singularity near $|y|^2 - 0$

13.9. NORMAL AND TIME ORDERED (CHRONOLOGICAL) PRODUCTS:

Now we discuss some mathematical preliminaries which will be needed in the later work. We start with by defiing the "Time Ordered product" of two operators.

The time ordered product of two Boson like operators A(x) and B(x') defined at two different space-time coordinates x and x' is defined as:

$$T\{A(x) B(x')\} = \begin{cases} A(x) B(x') & \text{if } x_0 > x_0' \\ B(x') A(x) & \text{if } x_0 < x_0' \end{cases} \dots (122)$$

For fermion like operators A(x) and B(x) it is defined as:

$$T \{A(x) B(x')\} = \begin{cases} A(x) B(x') & \text{if } x_0 > x_0' \\ -B(x') A(x) & \text{if } x_0 < x_0' \end{cases} ... (123)$$

In general, for Boson like operators:

$$T\{A(x) B(x')\} = \frac{1}{2} [A(x), B(x')]_{+} + \frac{1}{2} [A(x), B(x')] \in (x - x')$$

$$\dots(124)$$

where $\epsilon(x-x')$ is the signature factor

$$\epsilon (x-x') = \begin{cases} +1 & \text{if } x_0 > x_0' \\ -1 & \text{if } x_0 < x_0' \end{cases}$$
 ...(125)

Similarly, for fermion field,

$$T\{A(x) B(x')\} = \frac{1}{2} \in (x - x') [A(x), B(x')] + \frac{1}{2} [A(x), B(x')]$$

The idea of the "Normal Product" comes from the operation of the creation and the annihilation operators: viz

$$a \mid 0 \rangle = 0$$
 and $\langle 0 \mid a^{\dagger} = 0$...(127)

Thus, if we are given an arbitrary combination of these operators, the one which provides the maximum mathematical simplification is that in which all the destruction operators lie on the right of the creation operators. This type of product of the free particle creation and destruction operators in which all the creation operators stand to the left all the destruction operators called

as the normal product. If A is a destruction operator and B is a creation operator, then their normal product is given by:

$$N(AB) = N(BA) = BA$$
 for Boson like objects $\{ABA\} = -N(BA) = -BA$ for fermion like objects $\{ABA\} = -N(BA) = -BA$ for fermion like objects

As an explicit example, let us consider the real scalar field.

Then

$$N[\phi(x)\phi(x')] = N[\{\phi^{(+)}(x) + \phi^{(-)}(x)\} \{\phi^{(+)}(x') + \phi^{(-)}(x')\}]$$

$$= \phi^{(+)}(x)\phi^{(+)}(x') + \phi^{(-)}(x)\phi^{(+)}(x') + \phi^{(-)}(x)\phi^{(-)}(x')$$

$$+ \phi^{(-)}(x')\phi^{(+)}(x) \dots (129)$$

Also, for
$$x_0 > x_0'$$
 we have
$$T[\phi(x) \dot{\phi}(x')] = \phi(x) \phi(x') = [\phi^{(+)}(x) + \phi^{(-)}(x)] [\phi^{(+)}(x') + \phi^{(-)}(x')]$$

$$= \phi^{(+)}(x) \phi^{(+)}(x') + \phi^{(+)}(x) \phi^{(-)}(x') + \phi^{(-)}(x) \phi^{(+)}(x')$$

$$+ \phi^{(-)}(x) \phi^{(-)}(x') \dots (130)$$

Similarly, for $x_0 < x_0'$ we have

$$T[\phi(x) \phi(x')] = \phi^{(+)}(x') \phi^{(+)}(x) + \phi^{(+)}(x') \phi^{(-)}(x) + \phi^{(-)}(x') \phi^{(+)}(x) + \phi^{(-)}(x') \phi^{(-)}(x) + \phi^{(-)}(x') \phi^{(-)}(x) \qquad \dots (131)$$

$$T(\phi\phi') - N(\phi\phi') = \phi^{(+)}(x) \ \phi^{(-)}(x') - \phi^{(-)}(x') \ \phi^{(+)}(x)$$

$$= [\psi^{(+)}(x), \ \phi^{(-)}(x')] = i \triangle^{(+)}(x - x')$$
for $x_0 > x_0'$...(132)

and
$$T(\phi\phi')$$
 $N(\phi\phi') = \phi^{(+)}(x') \phi^{(-)}(x) - \phi^{(-)}(x) \phi^{(+)}(x')$

$$= -[\phi^{(-)}(x), \phi^{(+)}(x')] = -i \triangle^{(-)}(x - x')$$
for $x_0 < x_0'$... (133)

In eqns. (132) and (133) we have used the notation ϕ' for $\phi(x')$.

The difference of the time ordered product and the normal product of two operators is known as the Contractive Product, because it represents the contraction between two factors to represent the commutator or anticommutator which arise in going from a T-product to the N-product. We shall denote the contraction symbol by a line joining the two factors. Thus we write

$$T(\phi\phi') - N(\phi\phi') = \phi\phi' = \begin{cases} i\triangle^{(+)} (x - x') \text{ for } x_0 > x_0' \\ -i\triangle^{(-)} (x - x') \text{ for } x_0 < x_0' \end{cases}$$
(134)

It is left as an exercise for the readers to show that for the Dirac field:

$$T(\psi_{\alpha} \psi_{\beta'}) - N(\psi_{\alpha} \psi_{\beta'}) = \psi_{\alpha} \psi_{\beta'} = \begin{cases} iS_{\beta\alpha}^{(-)} (x - x') \text{ for } x_0 > x_0' \\ -iS_{\beta\alpha}^{(+)} (x - x') \text{ for } x_0 < x_0' \dots (135) \end{cases}$$

and

$$T(\psi_{\alpha} \ \bar{\psi}_{\beta}') - N(\psi_{\alpha} \ \bar{\psi}_{\beta}') = \psi_{\alpha} \ \bar{\psi}_{\beta}' = \begin{cases} iS_{\alpha\beta}^{(+)}(x - x') \text{ for } x_{0} > x_{0}' \\ -iS_{\alpha\beta}^{(-)}(x - x') \text{ for } x_{0} < x_{0}' \dots (136) \end{cases}$$

Since the function \triangle and S in (13), (135) and (136) are classical functions and not the operators, it is clear that a contracted pair of factors is a c-number. To this end we prove a very important theorem relating the T-product and the N-product due to Wick:

This theorem states that a T-product can be Wick's Theorem. decomposed into a unique sum of normal products as;

$$T(A_1 A_2 \dots A_n) = N(A_1 A_2 \dots A_n) + \sum_{i} N(A_1 A_2 \dots A_i A_{i+1} \dots A_n)$$

$$+ \sum_{i} \sum_{r} N(A_1 A_2 \dots A_i A_{i+1} \dots A_r A_{r+1} \dots A_n) + \dots + \dots \dots (137)$$

the second term on the r.h.s denotes all possible one pair contractions, the third term denotes all possible two pair contractions and so on till all the possibilities are exhausted.

Proof In order to prove the Wick's theorem, we need the following auxliary result, which we states as a lemma to the theorem.

Lemma. If B is an operator labelled with a time which is earlies than that of A_1, A_2, \ldots, A_n , then

$$N(A_1 A_2 \dots A_n) B = N(A_1 A_2 \dots A_n B) + \sum_{r=1}^n N(A_1 A_2 \dots A_r \dots A_n B);$$

$$N(A_1 A_2 \dots A_n B) = N(A_1 A_2 \dots A_n B) + \sum_{r=1}^n N(A_1 A_2 \dots A_r \dots A_n B);$$

where the line joining A_r and B denotes the contraction of A_r with B and $t_B < t_{Ar}$ for $r = 1, 2, \ldots, n$.

Proof of the Lemma. According to the definition of the . normal product, the lemma is still true if we regroup the operators $A_1, A_2, ..., A_n$, as long as the same regrouping is done of both the sides of the equation. We may, therefore, assume that the operators $A_1, A_2, ..., A_n$ are already in normal order with all creation operators standing to the left of all destruction operators. Now, we distinguish the following two cases:

B is an annihilation operators. Here we can have the

following probabilities:

All the A's are creation operator. $N(A_1A_2...A_n)B=(A_1A_2...A_n)B$

$$= (A_1 A_2 \dots A_n B)$$

$$= N (A_1 A_2 \dots A_n B) \dots (138)$$

Also, the contraction of a creation and a destruction operator, with the time label of the destruction operators earlier than that of the creation operator, can very easily be seen to vanish. We therefore, have

 $N(A_1A_2...A_r...A_n B) = 0$ for r = 1, 2, ..., n...(139)

From (138) and (1.9), we can see that the lemma is true for this case.

(b) Some of the A's are creation and some are destruction operators. Let A_1A_2 ... A_i be the creation, and A_{i+1} . A_{i+2} , ..., A_n be the destruction operator. Then, as we have assumed that all the A's are in the normal order, we have

$$N (A_1 A_2 \dots A_i \ A_{i+1} \dots A_n) B = (A_1 A_2 \dots A_i \ A_{i+1} \dots A_n) B$$

$$= (A_1 A_2 \dots A_i \ A_{i+1} \dots A_n B)$$

$$= N (A_1 A_2 \dots A_n B) \dots (140)$$

Also, from the argument of the previous possibility,

$$N(A_1A_2...A_r...A_n B)=0$$
 for $r=1, 2, ..., i$...(141)

and from the fact that the contraction of two destruction operators vanishes,

$$N(A_1A_2...A_r \ A_n \ B) = 0 \text{ for } r = i+1, i+2, ..., n ...(142)$$

From (140), (141) and (142), the lemma follows at once.

(c) In case all the A's are destruction operators, the lemma is trivial as a special case of possibility (b).

(II) B is a creation operator. Here also, we can have the following possibilities:

(a) All the A's are creation operator. The lemma is trivially proved in this case from the fact that the contraction of two creation operators vanishes

(b) The proof of the lemma in the case where some of the A's are creation and the others are the destruction operators is somewhat difficult. The worst is the case when all the A's are destruction operators. Thus it will be sufficient to prove the lemma in this worst case. We do it by induction, For n=1, we have

$$N(A_1) B = A_1 B = T(A_1 B)$$
 {: $t_B < t_{Ar}$ for all r }
= $[T(A_1 B) - N(A_1 S)] + N(A_1 B)$
= $A_1 B + N(A_1 B)$...(143)

Since A_1B is a complex number, therefore we have

$$N(A_1B)=A_1B.$$

Using it, from (143), we get

$$N(A_1)B=N(A_1B)+N(A_1B).$$

Thus the lemma is proved for n=1.

Now we assume that the lemma is true for k-factors, i.e.

$$N(A_1 A_2 ... A_k) B = N(A_1 A_2 ... A_k B) + \sum_{r=1}^k N(A_1 A_2 ... A_r ... A_k B) ... (144)$$

If we show that the lemma is also true for (k+1)-factors, then from the principle of induction it will be true in general. For it we multiply (144) by another destruction operator A_0 from left side, the time of A_0 is assumed to be later than that of B. Then,

$$A_0 N (A_1 A_2 . A_k) B = A_0 N (A_1 A_2 ... A_k B)$$

$$+A_0 \sum_{r=1}^{k} N (A_1 A_2 ... A_r ... A_k B) ... (145)$$

Now L.H.S. of (145) can be written as:

$$A_0N(A_1A_2...A_k) B=N(A_0 A_1A_2...A_k) B,$$

because A₀ and all the A's are destruction operators.

First term on the R.H.S. can be written as:

$$A_0 N (A_1 A_2 A_k B) = \delta_k A_0 B A_1 A_2 ... A_k,$$

where δ_k is the sign factor of the permutation of the fermion factors.

Since A_0 is labelled by time which is later than that of B, we have

$$A_0B = T(A_0B) = A_0B + N(A_0B)$$

$$= A_0B + \delta_0 BA_0$$

$$A_0N(A_1A_2...A_kB) = \delta_k (A_0B + \delta_0BA_0) A_1A_2...A_k.$$

$$= \delta_kN(A_0B A_1A_2...A_k) + \delta_k\delta_0N(BA_1 A_1...A_k)$$

Now we wish to take B at its proper place. In the first term, if we take B to its proper place, remembering that its contracted product is with A_0 it will pick up a signature factor δ_k in the process. Similarly, in the second term, the signature factor will be $\delta_k \delta_k$. Hence

$$A_0N(A_1A_2...A_kB) = \delta_k\delta_kN(A_0A_1A_2...A_kB) + \delta_0\delta_n\delta_0\delta_n N(A_3A_1...A_kB)$$

$$= N(A_0 A_1 A_2 ... A_k B) + N(A_0 A_1 ... A_k B)$$
Hence the R.H.S. of (145)
$$= N(A_0 A_1 A_2 ... A_k B) + N(A_0 A_1 ... A_k B)$$

$$+ A_0 \sum_{r=1}^{k} N(A_1 A_2 ... A_r ... A_k B)$$

$$= N(A_0 A_1 ... A_k B) + N(A_0 A_1 ... A_k B)$$

$$+ \sum_{r=1}^{k} N(A_0 A_1 A_2 ... A_r ... A_k B)$$

$$= N(A_0 A_1 ... A_k B) + \sum_{r=0}^{k} N(A_0 A_1 ... A_k ... A_k B)$$

Thus the eqn. (145) gives the equation:

$$N(A_0A_1...A_k) B = N(A_0A_1...A_kB)$$

$$+\sum_{r=0}^{k} N(A_0A_1...A_r...A_kB)$$
 ...(146)

Eqn. (146) shows that the lemma is true for (k+1) desruction operators, if it is true for k-operators, and hence it is true in general.

Now we are in a position to give the proof of the Wick's theorem, which is again by induction. For a single factor, the theorem is trivial. For two factors it is also true because by definition

$$T(A_1A_2) = N(A_1A_2) + A_1A_2$$
$$= N(A_1A_2) + N(A_1A_2)$$

Now assuming that the theorem is true for n factors, we prove it for (n+1) factors. For it we multiply (137) by A_{n+1} from right hand side, the time label of A_{n+1} is earlier than that of all the other A's. Then

$$T(A_{1}A_{2}...A_{n}) A_{n+1} = N(A_{1}A_{2}...A_{n}) A_{n+1} + \left[\sum_{i} N(A_{1}A_{2}...A_{i} A_{i+1}...A_{n})\right] A_{n+1} + \left[\sum_{i} \sum_{r} N(A_{1}A_{2}...A_{i} A_{i+1}...A_{r}A_{r+1}...A_{n})\right] A_{n+1} + ...$$

Since $t_{A_{n+1}} < t_{A_n}$, we can write the L.H.S. of the above as $T(A_1 A_2 ... A_n A_{n+1})$.

Using the above lemma, we have the first term on the R.H.S. as:

$$= N(A_1 A_2 A_3 ... A_{n+1}) + \sum_{r=1}^{n+1} N(A_1 A_2 ... A_r ... A_{n+1})$$

A particular term of the second term of R.H.S. is

$$N(A_1A_2A_3...A_n) A_{n+1} = N(A_1A_2A_3...A_n A_{n+1})$$

$$+\sum_{r=1}^{n+1} N(A_1 A_2 A_3 ... A_r ... A_{n+1})$$

Hence we get:

$$T(A_{1}A_{2}...A_{n+1}) = N(A_{1}...A_{n+1}) + \Sigma N(A_{1}A_{2}A_{3}...A_{n+1}) + \Sigma \Sigma N(A_{1}A_{2}A_{3}...A_{r+1}) + ...$$

Thus the theorem is true for (n+1) factors also and hence by induction it is true in general. This completes the proof of the Wick's theorem.

PROBLEMS

Problem 1. Give a representation of an arbitrary state vector for a Boson field in terms of a complete set of basis vectors in the FOCK-SPACE, together with an explicit calculation of the normalization for the basis states. Show how this representation incorporates Bose Statistics in the corresponding wave-functions.

Discuss briefly the modifications needed for a Fermi-field.

Sol. The space in which the number operator N_k is diagonalized is known as the Fock-space. The state-vectors of N_k in this space are built from the vacuum states, $| 0 \rangle$, in which there is no particle, by the operation of the creation operator $a\dagger$. For example, a state in which there is only one particle with momentum k_1 is given by

$$a_{k_1}^{\dagger} \mid 0 \rangle$$
 ...(i)

a state in which there are 15 particles with momentum k_1 and 20 particles with momentum k_2 can similarly be written as

and a general state with one particle of momentum k1, one particle

of momentum k2, ..., one particle of momentum kn can be written as

$$a_{k_1}^{\dagger} a_{k_2}^{\dagger} ... a_{k_n}^{\dagger} \mid 0 \rangle$$
 ...(iii)

All the states of the type (iii) form a complete set and hence we can represent any general state in terms of them. An arbitrary state vector $\phi(x)$ for the Boson field can be written in terms of the complete set (iii) as

$$\phi(x) = f_0 \mid 0 \rangle + \sum_{k_1} f(k_1) \, a_{k_1}^{\dagger} \mid 0 \rangle + \sum_{k_1, k_2} f(k_1, k_2) \, a_{k_1}^{\dagger} \, a_{k_2}^{\dagger} \mid 0 \rangle + \dots + \sum_{k_1, k_2, \dots, k_n} f(k_1, k_2, \dots, k_n) \, a_{k_1}^{\dagger} \, a_{k_2}^{\dagger} \dots a_{k_n}^{\dagger} \mid 0 \rangle + \dots \quad \text{(iv)}$$

Here f's are c-number functions depending on the characteristics of the particles (momenta and spins) and on the positions of the particles. They describe the spatial dependence of the system and the distribution of particles over the various possible individual states. The summation is over all possible momenta and spins of all particles.

The successive terms on the r.h.s. of (iv) are the no particle, one particle, two particles..., states. Let us now properly normalize these basis states.

The no particle state is clearly normalized. For one particle state we have

$$\langle 0 \mid a_{k_{1}}^{\dagger} a_{k_{1}}^{\dagger} \mid 0 \rangle = \langle 0 \mid (a_{k_{1}}^{\dagger} a_{k_{1}}^{\dagger} - a_{k_{1}}^{\dagger} a_{k_{1}}^{\dagger}) \mid 0 \rangle$$

$$\{ :: a_{k_{1}}^{\dagger} \mid 0 \rangle = 0 \}$$

$$= \langle 0 \mid [a_{k_{1}}, a_{k_{1}}^{\dagger}] \mid 0 \rangle = 1$$

Thus it is also properly normalized. For the particles state, we have

$$\begin{array}{l} \langle 0 \mid a_{k_{2}} \, a_{k_{1}} \, a_{k_{1}}^{\dagger} \, a_{k_{2}}^{\dagger} \mid 0 \rangle = \langle 0 \mid a_{k_{2}} \, (1 + a_{k_{1}}^{\dagger} \, a_{k_{1}} \,) \, a_{k_{2}}^{\dagger} \mid 0 \rangle \\ & = \langle 0 \mid a_{k_{2}} \, a_{k_{2}}^{\dagger} \mid 0 \rangle \\ & + \langle 0 \mid a_{k_{2}} \, a_{k_{1}}^{\dagger} \, a_{k_{1}} \, a_{k_{2}}^{\dagger} \mid 0 \rangle \\ & = 1 + \langle 0 \mid (\delta_{k_{2} \, k_{1}} \, + a_{k_{1}}^{\dagger} \, a_{k_{2}} \,) \, (\delta_{k_{1} k_{2}} \, + a_{k_{2}}^{\dagger} \, a_{k_{1}} \,) \mid 0 \rangle \\ & = 1 + \delta_{k_{2} k_{1}} \, \delta_{k_{1} k_{2}} \quad \{ :: \quad a_{k_{2}} \mid 0 \rangle = a_{k_{1}} \mid 0 \rangle = 0 \} \\ & = 1 + 1 = 2 \, ! \end{array}$$

Hence the normalization constant for two particle state is

Similarly, it can be shown that the normalization constant for three particle state is $\frac{1}{\sqrt{(3)!}}$, and in general, the normalization constant for the *n* particle basis state will be $\frac{1}{\sqrt{(n)!}}$. Hence the arbitrary state vector $\phi(x)$ can be expressed in terms of the normalized basis vectors in the Fock-space as

$$\phi(1) \qquad \phi(1) \qquad \int_{\sqrt{(1)!}} \int_{k_{1}}^{f(k_{1})} a_{k_{1}}^{\dagger} | 0 \rangle$$

$$\phi(1, 2) \qquad \frac{1}{\sqrt{(2)!}} \sum_{k_{2}}^{f(k_{1}, k_{2})} a_{k_{1}}^{\dagger} a_{k_{2}}^{\dagger} | 0 \rangle$$

$$\psi(1, 2, ..., n) \qquad \frac{1}{\sqrt{(n)!}} \sum_{k_{1}, k_{2}, ..., k_{n}} \int_{k_{1}}^{f(k_{1}, k_{2}, ..., k_{n})} a_{k_{1}}^{\dagger} a_{k_{2}}^{\dagger} ... a_{k_{n}}^{\dagger} | 0 \rangle$$

In order to show that this representation is for Bosons operators, we note that the operators $a_{k_1}^{\dagger}$, $a_{k_2}^{\dagger}$, ..., $a_{k_n}^{\dagger}$ etc. commutes with each other and hence an interchange of these does not make any difference to the representation, i.e., the state remains unchanged. On the other hand, interchange of any pair of these particles. Thus we can say that the states of this representation are symmetric under the interchange of particles and this is the basic requirement of the Bose-Statistics.

The description of the fermi field is quite similar to that of the Bose field. The situation, in fact, is simpler because the property of antisymmetrized basis vectors is such that not more than one particle can be there in any state.

The zero particle and one particle states are the same as in the case of Boson field. The only difference here is that we have to use the anticommutators in place of the commutators.

Problem 2. Show that for a Dirac field

(i) $T[\psi_{\alpha}(x)\psi_{\beta}(x')]-N[\psi_{\alpha}(x)\psi_{\beta}(x')]=0$

(ii) $\Sigma \Sigma (\gamma_{\mu})_{\alpha\beta} \frac{1}{2} [\bar{\psi}_{\alpha}(x), \psi_{\beta}(x)] = \Sigma \Sigma (\gamma_{\mu})_{\alpha\beta} N (\bar{\psi}_{\alpha} \psi_{\beta}).$

Sol. (i) We write,

 $\psi_{\alpha}(x) \psi_{\beta}(x') = (\psi_{\alpha}^{(+)} + \psi_{\alpha}^{(-)}) (\psi_{\beta}^{(+)} + \psi_{\beta}^{(-)})$

 $= \psi_{\alpha}(^{+}) \psi_{\beta}(^{+}) + \psi_{\alpha}(^{+}) \psi_{\beta}(^{-}) + \psi_{\alpha}(^{-}) \psi_{\beta}(^{+}) + \psi_{\alpha}(^{-}) \psi_{\beta}(^{-})$

 $N \left[\psi_{\alpha}(x) \psi_{\beta}(x') \right] = \psi_{\alpha}^{(+)}(x) \psi_{\beta}^{(+)}(x') - \psi_{\beta}^{(-)}(x') \psi_{\alpha}^{(+)}(x)$ $+\psi_{\alpha}^{(-)}(x)\psi_{\beta}^{(+)}(x')+\psi_{\alpha}^{(-)}(x)\psi_{\beta}^{(-)}(x')...(i)$

For $x_0 > x'_0$,

 $T \left[\psi_{\alpha} (x) \psi_{\beta} (x') \right] = \psi_{\alpha}^{(+)} (x) \psi_{\beta}^{(+)} (x') + \psi_{\alpha}^{(+)} (x) \psi_{\beta}^{(-)} (x')$ $+\psi_{a}^{(-)}(x)\psi_{g}^{(+)}(x')+\psi_{a}^{(-)}(x)\psi_{g}^{(-)}(x')\dots$ (ii)

Hence using eqn. (110), we have

 $T[\psi_{\alpha}(x) \psi_{\beta}(x')] - N[\psi_{\alpha}(x) \psi_{\beta}(x')] = [\psi_{\alpha}^{(+)}(x), \psi_{\beta}^{(-)}(x')]_{+} = 0.$ For $x_0 < x_0'$,

 $T \left[\psi_{\alpha} (x) \psi_{\beta} (x') \right] = -\psi_{\beta}^{(+)} (x') \psi_{\alpha}^{(+)} (x) - \psi_{\beta}^{(-)} (x') \psi_{\alpha}^{(+)} (x) \right]_{+}$ $-\psi_{\beta}^{(+)}(x')\psi_{\alpha}^{(-)}(x)-\psi_{\beta}^{(-)}(x')\psi_{\alpha}^{(-)}(x)$...(iii)

Hence, we have $T \left[\psi_{\alpha} (x) \psi_{\beta} (x') - N (\psi_{\alpha} (x) \psi_{\beta} (x')) \right] = - \left[\psi_{\beta}^{(+)} (x'), \phi_{\alpha}^{(+)} (x) \right]_{+}$ $-[\psi_{\beta}^{(+)}(x'),\psi_{\alpha}^{(-)}(x)]_{+}-[\psi_{\beta}^{(-)}(x'),\psi_{\alpha}^{(-)}(x)]=0.$

Thus the result (i) is true for both the cases.

(ii) To prove this result. we have

 $\frac{1}{2} \left[\psi_{\alpha}(x), \psi_{\beta}(x) \right] N \left[\psi_{\alpha}(x) \psi_{\beta}(x) \right] = \frac{1}{2} \left(\psi_{\alpha}(-) + \psi_{\alpha}(-) \right) \left(\psi_{\beta}(+) + \psi_{\beta}(-) \right)$ $-\frac{1}{2} \left(\psi_{\beta}^{(+)} + \psi_{\beta}^{(-)} \right) \left(\bar{\psi}_{\alpha}^{(+)} + \bar{\psi}_{\alpha}^{(-)} \right) - N \left[\left(\bar{\psi}_{\alpha}^{(+)} + \bar{\psi}_{\alpha}^{(-)} \right) \left(\bar{\psi}_{\beta}^{(+)} + \psi_{\beta}^{(-)} \right) \right]$ $= \frac{1}{2} \left(\bar{\psi}_{\alpha}^{(+)} \psi_{\beta}^{(+)} + \bar{\psi}_{\alpha}^{(+)} \psi_{\beta}^{(-)} + \bar{\psi}_{\alpha}^{(-)} + \bar{\psi}_{\alpha}^{(-)} \psi_{\beta}^{(-)} + \bar{\psi}_{\alpha}^{(-)} \psi_{\beta}^{(-)} \right)$ $-\frac{1}{2} \left(\psi_{\beta}^{(+)} \bar{\psi}_{\alpha}^{(+)} + \psi_{\beta}^{(+)} \bar{\psi}_{\alpha}^{(-)} + \psi_{\beta}^{(-)} \bar{\psi}_{\alpha}^{(-)} + \psi_{\beta}^{(-)} \bar{\psi}_{\alpha}^{(-)} \right)$ $-(\bar{\psi}_{\alpha}^{(+)}\psi_{\beta}^{(+)}-\psi_{\beta}^{(-)}\bar{\psi}_{\alpha}^{(+)}+\bar{\psi}_{\alpha}^{(-)}\psi_{\beta}^{(+)}+\bar{\psi}_{\alpha}^{(+)}+\bar{\psi}_{\alpha}^{(+)}\psi_{\beta}^{(-)})$ $= \frac{1}{2} \bar{\psi}_{\alpha}^{(+)} \psi_{\beta}^{(-)} - \frac{1}{2} (\psi_{\beta}^{(+)} \bar{\psi}_{\alpha}^{(+)} + \psi_{\beta}^{(+)} \bar{\psi}_{\alpha}^{(+)}) + \psi_{\beta}^{(+)} \bar{\psi}_{\alpha}^{(-)} + \psi_{\beta}^{(-)} \bar{\psi}_{\alpha}^{(-)})$ $-\frac{1}{2} \left(\bar{\psi}_{\alpha}^{(+)} \psi_{\beta}^{(+)} - \psi_{\beta}^{(-)} \bar{\psi}_{\alpha}^{(+)} + \bar{\psi}_{\alpha}^{(-)} \psi_{\beta}^{(+)} + \bar{\psi}_{\alpha}^{(-)} \psi_{\beta}^{(+)} + \bar{\psi}_{\alpha}^{(-)} \psi_{\beta}^{(-)} \right)$

= $-\frac{1}{2} \left[\psi_{\alpha}, \psi_{\beta}^{(+)} \right]_{+} + \frac{1}{2} \left[\psi_{\beta}^{(-)}, \overline{\psi}_{\alpha}^{(+)} \right]_{+}$

 $-\frac{1}{2} \left[\psi_{\beta}^{(+)}, \overline{\psi}_{\alpha}^{(+)} \right]_{+} - \frac{1}{2} \left[\psi_{\beta}^{(-)}, \overline{\psi}_{\alpha}^{(-)} \right]_{+}$ $= -\frac{1}{2} S_{\beta\alpha}^{(+)}(0) + \frac{1}{2} S_{\beta\alpha}^{(-)}(0).$

...(iv)

Now

$$i\triangle^{(\pm)} = \pm \frac{1}{(2\pi)^3} \int \frac{d^3k}{2\omega_k} e^{\pm ik\cdot y}$$

Y

$$iS_{\beta\alpha}^{(\pm)} = (m - \mathcal{J})_{\beta\alpha} i \triangle^{(\pm)}$$

$$1 \quad \int d^3k$$

 $=\frac{1}{(2\pi)^3}\int \frac{d^3k}{2\omega_k} (\pm m-ik)_{\beta\alpha} e^{\pm i\hbar\cdot y}.$

Using (v) in (iv), we get

 $(\gamma_{\mu})_{\alpha\beta}$ { $\frac{1}{2}$ [$\overline{\psi}_{\alpha}(x), \psi_{\beta}(x)$]—N [$\overline{\psi}_{\alpha}(x) \psi_{\beta}(x)$]}

$$= \frac{Lt}{y \to 0} - \frac{m}{(2\pi)^3} \int \frac{d^3k}{2\omega_k} \, \delta_{\beta\alpha} \, e^{\pm ik \cdot y} \, (\gamma_\mu)_{\alpha\beta}.$$

$$\sum_{\alpha} \sum_{\beta} (\gamma_{\mu})_{\alpha\beta} \frac{1}{2} \left[\overline{\psi}_{\alpha} (x), \psi_{\beta} (x) \right] - \sum_{\alpha} \sum_{\beta} (\gamma_{\mu})_{\alpha\beta} N \left(\overline{\psi}_{\alpha} \psi_{\beta} \right)$$

$$= -m T_{race} (\gamma_{\mu}) = 0$$

and hence, we have

$$\sum_{\alpha} \sum_{\beta} (\gamma_{\mu})_{\alpha\beta} \frac{1}{2} \left[\bar{\psi}_{\alpha} (x), \psi_{\beta} (x) \right] = \sum_{\alpha} \sum_{\beta} (\gamma_{\mu})_{\alpha\beta} N (\bar{\psi}_{\alpha} \psi_{\beta})$$

Problem 3. Show that for a free Dirac field $\psi_{\alpha}(x)$,

$$T[\psi_x(x)\overline{\psi}_\beta(x')]-N[\psi_x(x)\overline{\psi}_\beta(\overline{x'})]$$

$$=\langle 0 \mid T \left[\psi_{\alpha} \left(x \right) \psi_{\beta} \left(x' \right) \right] \mid 0 \rangle$$

and find a four-dimensional integral representation for the right hand side.

Similar to problem 3, here also we can easily show that

$$T \left[\psi_{\alpha} \left(x \right) \overline{\psi}_{\beta} \left(x' \right) \right] - N \left[\psi_{\alpha} \left(x \right) \overline{\psi}_{\beta} \left(x' \right) \right]$$

$$= \langle 0 \mid T \left(\psi_{\alpha} \left(x \right) \overline{\psi}_{\beta} \left(x' \right) \mid 0 \rangle$$

$$= \begin{cases} iS_{\alpha\beta}^{(+)} \left(x - x' \right) & \text{for } x_{0} > x_{0}' \\ -iS_{\alpha\beta}^{(-)} \left(x - x' \right) & \text{for } x_{0} < x_{0}' \end{cases}$$

In order to find the integral representation, we have

$$S_{\alpha\beta}^{(-)}(x-x') = (m-\tilde{z}_y)_{z\beta} \triangle^{(-)}(y)$$

$$= -(m-\tilde{z}_y)_{\alpha\beta} \frac{1}{(2\pi)^4} \int \frac{d^4k}{k^2+m^2} e^{iky}$$

$$(\partial_{y} + m) S_{\alpha\beta}^{(-)}(x - x')$$

$$= -(m^{2} - \partial^{2}y) \frac{1}{(2\pi)^{4}} \int \frac{d^{4}k}{k^{2} + m^{2}} e^{ik \cdot y}$$

$$= -\frac{1}{(2\pi)^{4}} \int d^{4}k \ e^{ik \cdot y} = -\delta^{4}(y)$$

$$= -\delta^{4}(x - x')$$

Or

$$(\tilde{c}_y + m) i S_{\alpha\beta}^{(-)} (x-x') = -i \delta^4 (x-x')$$

Thus, in the case of free Dirac field,

$$i S_{\alpha\beta}^{(-)}(x-x')$$

plays the role of the Feynman's propagator.

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